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PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

NEWS	1		Web Page URLs for STN Seminar Schedule - N. America
NEWS	2		"Ask CAS" for self-help around the clock
NEWS	3	DEC 23	New IPC8 SEARCH, DISPLAY, and SELECT fields in USPATFULL/ USPAT2
NEWS	4	JAN 13	IPC 8 searching in IFIPAT, IFIUDB, and IFICDB
NEWS	5	JAN 13	New IPC 8 SEARCH, DISPLAY, and SELECT enhancements added to INPADOC
NEWS	6	JAN 17	Pre-1988 INPI data added to MARPAT
NEWS	7	JAN 17	IPC 8 in the WPI family of databases including WPIFV
NEWS	8	JAN 30	Saved answer limit increased
NEWS	9	FEB 21	STN AnaVist, Version 1.1, lets you share your STN AnaVist visualization results
NEWS	10	FEB 22	The IPC thesaurus added to additional patent databases on STN
NEWS	11	FEB 22	Updates in EPFULL; IPC 8 enhancements added
NEWS	12	FEB 27	New STN AnaVist pricing effective March 1, 2006
NEWS	13	FEB 28	MEDLINE/LMEDLINE reload improves functionality
NEWS	14	FEB 28	TOXCENTER reloaded with enhancements
NEWS	15	FEB 28	REGISTRY/ZREGISTRY enhanced with more experimental spectral property data
NEWS	16	MAR 01	INSPEC reloaded and enhanced
NEWS	17	MAR 03	Updates in PATDPA; addition of IPC 8 data without attributes
NEWS	18	MAR 08	X.25 communication option no longer available after June 2006
NEWS	19	MAR 22	EMBASE is now updated on a daily basis
NEWS	20	APR 03	New IPC 8 fields and IPC thesaurus added to PATDPAFULL
NEWS	21	APR 03	Bibliographic data updates resume; new IPC 8 fields and IPC thesaurus added in PCTFULL
NEWS	22	APR 04	STN AnaVist $500 visualization usage credit offered
NEWS	23	APR 12	LINSPEC, learning database for INSPEC, reloaded and enhanced
NEWS	24	APR 12	Improved structure highlighting in FQHIT and QHIT display in MARPAT
NEWS	25	APR 12	Derwent World Patents Index to be reloaded and enhanced during second quarter; strategies may be affected

NEWS EXPRESS FEBRUARY 15 CURRENT VERSION FOR WINDOWS IS V8.01a,
CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
AND CURRENT DISCOVER FILE IS DATED 19 DECEMBER 2005.
V8.0 AND V8.01 USERS CAN OBTAIN THE UPGRADE TO V8.01a AT
http://download.cas.org/express/v8.0-Discover/

NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS LOGIN	Welcome Banner and News Items
NEWS IPC8	For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that

specific topic.

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* * * * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 14:34:11 ON 13 APR 2006

=> file registry

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 14:34:19 ON 13 APR 2006
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 11 APR 2006 HIGHEST RN 880129-32-8
DICTIONARY FILE UPDATES: 11 APR 2006 HIGHEST RN 880129-32-8

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 6, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

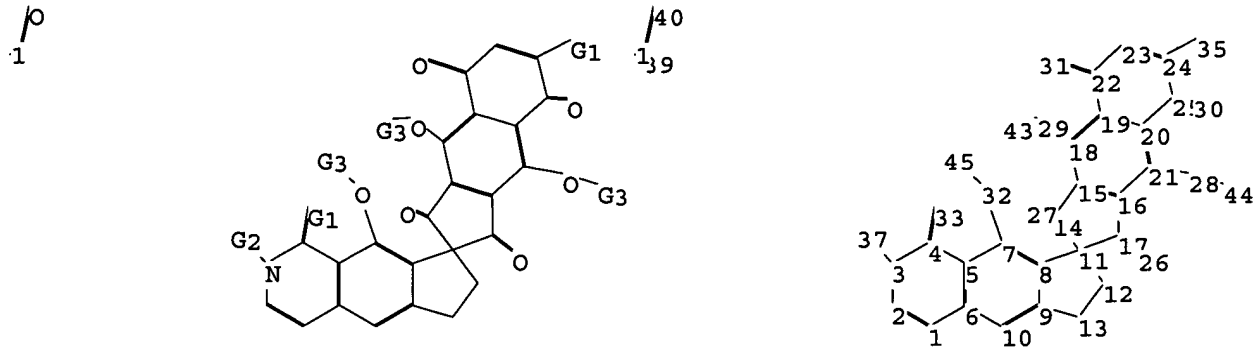
****
* *
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added, *
* effective March 20, 2005. A new display format, IDERL, is now *
* available and contains the CA role and document type information. *
* *
****

Structure search iteration limits have been increased. See HELP SLIMITS for details.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=>
Uploading C:\Program Files\Stnexp\Queries\10509066.str



chain nodes :
26 27 28 29 30 31 32 33 35 37 39 40 43 44 45
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25
chain bonds :
3-37 4-33 7-32 14-27 17-26 18-29 21-28 22-31 24-35 25-30 28-44 29-43 32-45 39-40
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 8-11 9-10 9-13 11-12 11-14 11-17 12-13 14-15 15-16 15-18 16-17 16-21 18-19 19-20 19-22 20-21 20-25 22-23 23-24 24-25
exact/norm bonds :
1-2 1-6 2-3 3-4 3-37 4-5 4-33 7-32 8-11 9-13 11-12 11-14 11-17 12-13 14-15 14-27 16-17 17-26 18-29 19-22 20-25 21-28 22-23 22-31 23-24 24-25 24-35 25-30 28-44 29-43 32-45 39-40
normalized bonds :
5-6 5-7 6-10 7-8 8-9 9-10 15-16 15-18 16-21 18-19 19-20 20-21

G1:O,S,N

G2:H,Cb,Ak

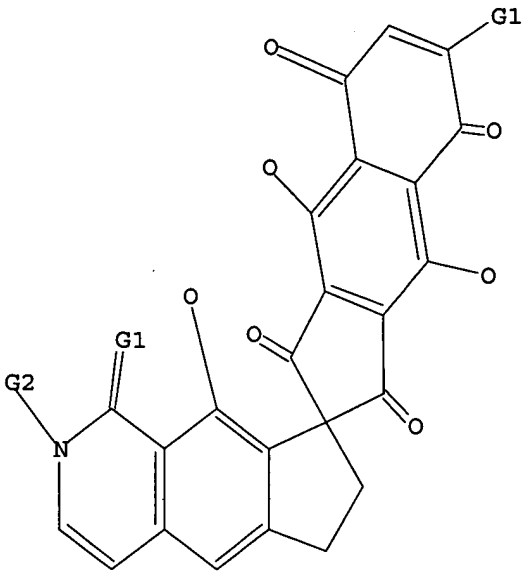
G3:H,Ak,[*1]

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS 31:CLASS 32:CLASS 33:CLASS 35:CLASS 37:CLASS 39:CLASS 40:CLASS 43:CLASS 44:CLASS 45:CLASS

L1 STRUCTURE UPLOADED

10509066

```
=> d l1
L1 HAS NO ANSWERS
L1                STR
```



G1 O,S,N

G2 H,Cb,Ak

Structure attributes must be viewed using STN Express query preparation.

```
=> s l1
SAMPLE SEARCH INITIATED 14:34:47 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -       20 TO ITERATE

100.0% PROCESSED       20 ITERATIONS                              12 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:          132 TO      668
PROJECTED ANSWERS:              33 TO      447

L2            12 SEA SSS SAM L1

=> s l1 ful
FULL SEARCH INITIATED 14:34:51 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -      488 TO ITERATE

100.0% PROCESSED      488 ITERATIONS                             243 ANSWERS
SEARCH TIME: 00.00.07

L3           243 SEA SSS FUL L1

=> file caplus
COST IN U.S. DOLLARS                              SINCE FILE      TOTAL
                                                     ENTRY    SESSION
FULL ESTIMATED COST                                 166.94     167.15
```

FILE 'CAPLUS' ENTERED AT 14:35:02 ON 13 APR 2006
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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FILE COVERS 1907 - 13 Apr 2006 VOL 144 ISS 16
FILE LAST UPDATED: 12 Apr 2006 (20060412/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply.
They are available for your review at:

http://www.cas.org/infopolicy.html

=> s l3
L4 121 L3

=> file registry

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	2.76	169.91

FILE 'REGISTRY' ENTERED AT 14:38:26 ON 13 APR 2006
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 11 APR 2006 HIGHEST RN 880129-32-8
DICTIONARY FILE UPDATES: 11 APR 2006 HIGHEST RN 880129-32-8

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 6, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

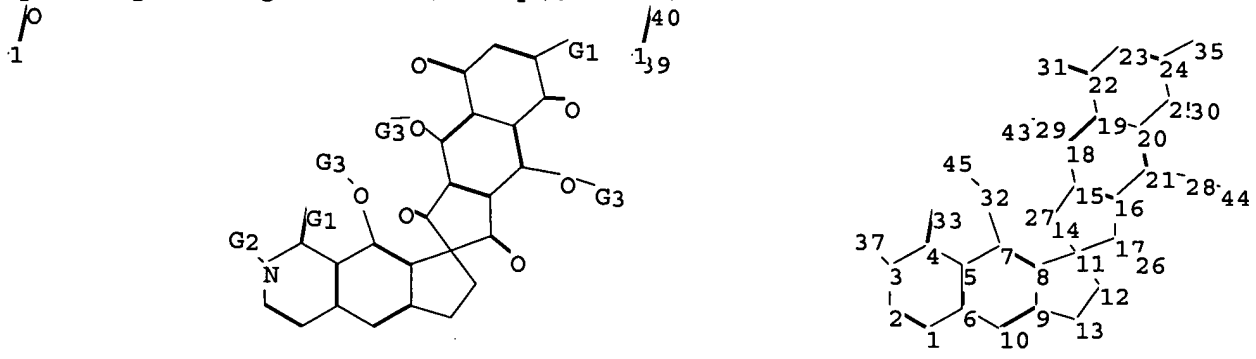
```
**********************************************************************
*                                                                    *
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added,    *
* effective March 20, 2005.  A new display format, IDERL, is now     *
* available and contains the CA role and document type information.  *
*                                                                    *
**********************************************************************
```

Structure search iteration limits have been increased. See HELP SLIMITS for details.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=>
Uploading C:\Program Files\Stnexp\Queries\10509066.str



chain nodes :
26 27 28 29 30 31 32 33 35 37 39 40 43 44 45
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25
chain bonds :
3-37 4-33 7-32 14-27 17-26 18-29 21-28 22-31 24-35 25-30 28-44 29-43 32-45 39-40
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 8-11 9-10 9-13 11-12 11-14 11-17 12-13 14-15 15-16 15-18 16-17 16-21 18-19 19-20 19-22 20-21 20-25 22-23 23-24 24-25
exact/norm bonds :
1-2 1-6 2-3 3-4 3-37 4-5 4-33 7-32 8-11 9-13 11-12 11-14 11-17 12-13 14-15 14-27 16-17 17-26 18-29 19-22 20-25 21-28 22-23 22-31 23-24 24-25 24-35 25-30 28-44 29-43 32-45 39-40
normalized bonds :
5-6 5-7 6-10 7-8 8-9 9-10 15-16 15-18 16-21 18-19 19-20 20-21

G1:O,S,N

G2:H,Cb,Ak

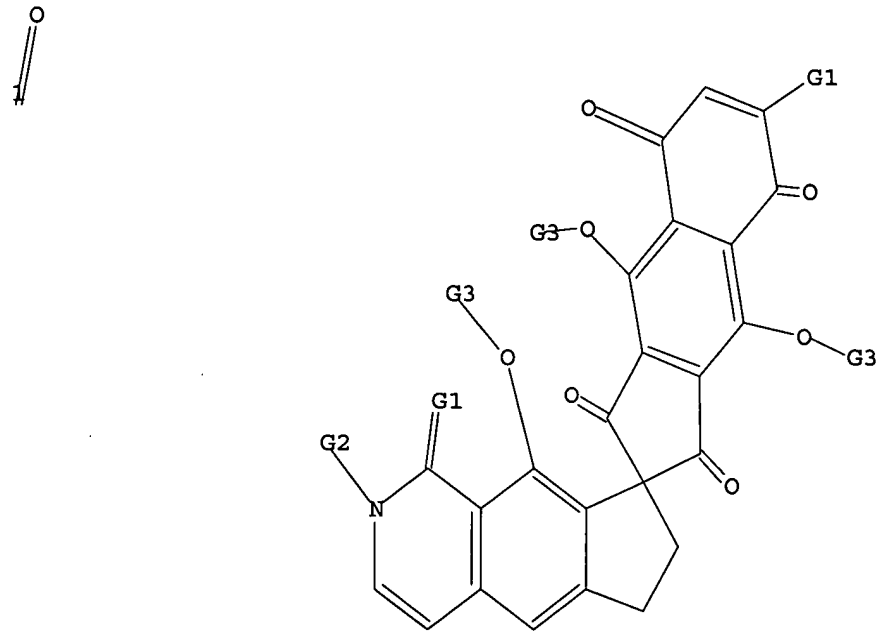
G3:H,Ak,[*1]

10509066

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom
20:Atom 21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:CLASS 27:CLASS 28:CLASS
29:CLASS 30:CLASS 31:CLASS 32:CLASS 33:CLASS 35:CLASS 37:CLASS 39:CLASS
40:CLASS 43:CLASS 44:CLASS 45:CLASS

L5 STRUCTURE UPLOADED

=> d l5
L5 HAS NO ANSWERS
L5 STR



G1 O,S,N

G2 H,Cb,Ak

G3 H,Ak,[@1]

Structure attributes must be viewed using STN Express query preparation.

=> s l5
SAMPLE SEARCH INITIATED 14:38:49 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 20 TO ITERATE

100.0% PROCESSED 20 ITERATIONS 12 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 132 TO 668
PROJECTED ANSWERS: 33 TO 447

L6 12 SEA SSS SAM L5

=> s l5 ful
FULL SEARCH INITIATED 14:38:55 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 488 TO ITERATE

100.0% PROCESSED 488 ITERATIONS 241 ANSWERS
SEARCH TIME: 00.00.01

L7 241 SEA SSS FUL L5

=> file caplus
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 166.94 336.85

FILE 'CAPLUS' ENTERED AT 14:39:04 ON 13 APR 2006
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907 - 13 Apr 2006 VOL 144 ISS 16
FILE LAST UPDATED: 12 Apr 2006 (20060412/ED)

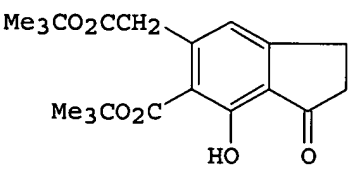
Effective October 17, 2005, revised CAS Information Use Policies apply.
They are available for your review at:

http://www.cas.org/infopolicy.html

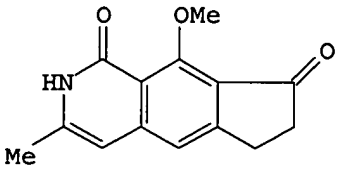
=> s l7
L8 121 L7

=> d abs bib hitstr 100-121

L8 ANSWER 100 OF 121 CAPLUS COPYRIGHT 2006 ACS on STN
GI



I



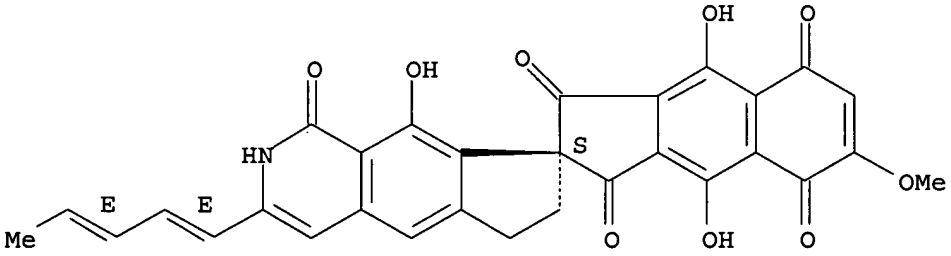
II

AB The polyketide condensation of Me3CO2C(CH2CO)2CH2CH2(COCH2)2CO2CMe3,

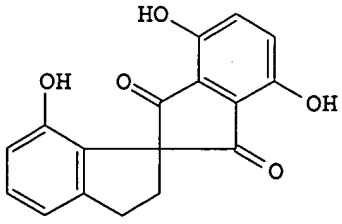
prepared from MeCOCH2CO2CMe3 and MeO2CCH2CH2CO2Me, gave the indanone I. I was converted to the cyclopentaisoquinoline fragment II of fredericamycin in 4 steps.

AN 1987:423138 CAPLUS
DN 107:23138
TI Strategies and intermediates for fredericamycin A synthesis. A 3-substituted 9-alkoxycyclopenta[g]isoquinoline-1,8(2H)-dione
AU Parker, Kathlyn A.; Breault, Gloria A.
CS Dep. Chem., Brown Univ., Providence, RI, 02912, USA
SO Tetrahedron Letters (1986), 27(33), 3835-8
CODEN: TELEAY; ISSN: 0040-4039
DT Journal
LA English
OS CASREACT 107:23138
IT **80455-68-1P**, Fredericamycin A
RL: SPN (Synthetic preparation); PREP (Preparation)
(cyclopentaisoquinolinedione fragment of, preparation of)
RN 80455-68-1 CAPLUS
CN Spiro[2H-benz[f]indene-2,8'-[8H]cyclopent[g]isoquinoline]-1,1',3,5,8(2'H)-pentone, 6',7'-dihydro-4,9,9'-trihydroxy-6-methoxy-3'-[(1E,3E)-1,3-pentadienyl]-, (2S)- (9CI) (CA INDEX NAME)

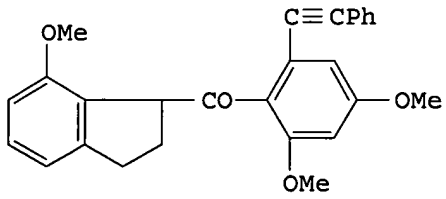
Absolute stereochemistry.
Double bond geometry as shown.



L8 ANSWER 101 OF 121 CAPLUS COPYRIGHT 2006 ACS on STN
GI



I

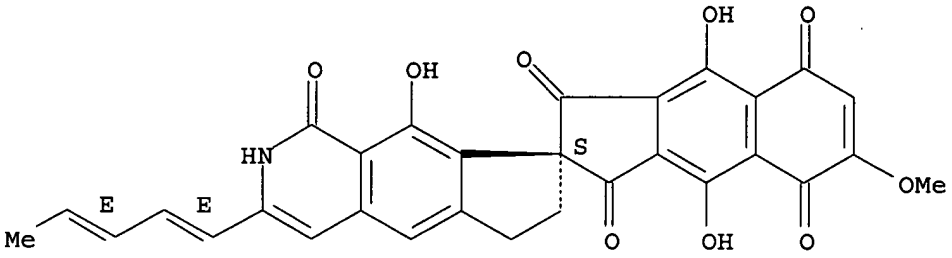


II

AB The spiro compound I, that represents the central 4 rings of the antitumor agent, fredericamycin A, has been synthesized by using the general technique of radical spirocyclization. The key intermediate II was assembled from 7-methoxyindancarboxaldehyde and 2,3,6-Br(MeO)2C6H2C.tplbond.CPh, followed by oxidation of the resulting alc. Phenylselenylation of II and treatment with Ph3SnH gave the spirocycle which on ozonolysis and deprotection with BBr3 gave I.
AN 1987:176011 CAPLUS

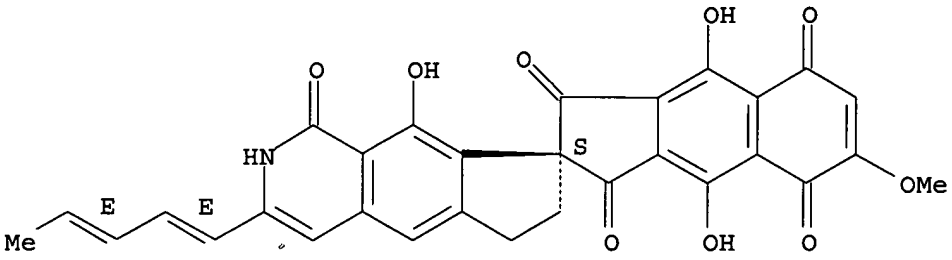
DN 106:176011
TI Radical spirocyclization: synthesis of an appropriately oxygenated spiro compound related to the antitumor antibiotic fredericamycin A
AU Clive, Derrick, L. J.; Angoh, A. Gaetan; Bennett, Sharon M.
CS Dep. Chem., Univ. Alberta, Edmonton, AB, T6G 2G2, Can.
SO Journal of Organic Chemistry (1987), 52(7), 1339-42
CODEN: JOCEAH; ISSN: 0022-3263
DT Journal
LA English
OS CASREACT 106:176011
IT **80455-68-1P**, Fredericamycin A
RL: SPN (Synthetic preparation); PREP (Preparation)
(spirobiindan ring system of, preparation of)
RN 80455-68-1 CAPLUS
CN Spiro[2H-benz[f]indene-2,8'-[8H]cyclopent[g]isoquinoline]-1,1',3,5,8(2'H)-pentone, 6',7'-dihydro-4,9,9'-trihydroxy-6-methoxy-3'-[(1E,3E)-1,3-pentadienyl]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



L8 ANSWER 102 OF 121 CAPLUS COPYRIGHT 2006 ACS on STN
AB Several approaches to trialkoxyphthalic acid derivs., potential intermediates in a fredericamycin synthesis, were tested. Sequences based on a Diels-Alder/retro Diels-Alder reaction, a cyanide addition to a quinone, an Elbs oxidation, and an amide-directed ortho-lithiation are discussed in terms of length, yields, convenience, and the versatility of the product of each.
AN 1987:66847 CAPLUS
DN 106:66847
TI Evaluation of some preparations of trialkoxyphthalic acid derivatives
AU Parker, Kathlyn A.; Spero, Denice M.; Koziski, Kathleen A.
CS Dep. Chem., Brown Univ., Providence, RI, 02912, USA
SO Journal of Organic Chemistry (1987), 52(2), 183-8
CODEN: JOCEAH; ISSN: 0022-3263
DT Journal
LA English
OS CASREACT 106:66847
IT **80455-68-1**, Fredericamycin A
RL: RCT (Reactant); RACT (Reactant or reagent)
(trialkoxyphthalic acid intermediates for, preparation of)
RN 80455-68-1 CAPLUS
CN Spiro[2H-benz[f]indene-2,8'-[8H]cyclopent[g]isoquinoline]-1,1',3,5,8(2'H)-pentone, 6',7'-dihydro-4,9,9'-trihydroxy-6-methoxy-3'-[(1E,3E)-1,3-pentadienyl]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



L8 ANSWER 103 OF 121 CAPLUS COPYRIGHT 2006 ACS on STN
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Stable fredericamycin A derivs. I (R = H, C1-4 alkyl; R1 = C1-4 alkyl), useful as neoplasm inhibitors, were prepared Thus, fredericyamin A (II) was reduced over 10% Pd/C in THF at room temperature for 10 h, then stirred with Ac2O for 1 h to give 80% III. III was heated with MeI and Ag2O in Me2CO for 1 h to give 56.3% I (R = R1 = Me), whose i.p. administration prolonged the lives of mice transplanted with Ehrlich cancer cells (5 + 106 cells/animal) in a dose dependent manner. A saline solution of III was more stable than that of II.

AN 1987:49879 CAPLUS

DN 106:49879

TI Fredericamycin A derivatives

IN Hasegawa, Hiroshi; Yokoi, Koichi; Narita, Masa; Asaoka, Takemitsu; Kukita, Kenichi; Ishizeki, Seiji; Nakajima, Toshiaki

PA S. S. Pharmaceutical Co., Ltd., Japan

SO Jpn. Kokai Tokkyo Koho, 6 pp.
CODEN: JKXXAF

DT Patent

LA Japanese

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 61044867	A2	19860304	JP 1984-166283	19840808
	JP 03004548	B4	19910123		
PRAI	JP 1984-166283		19840808		

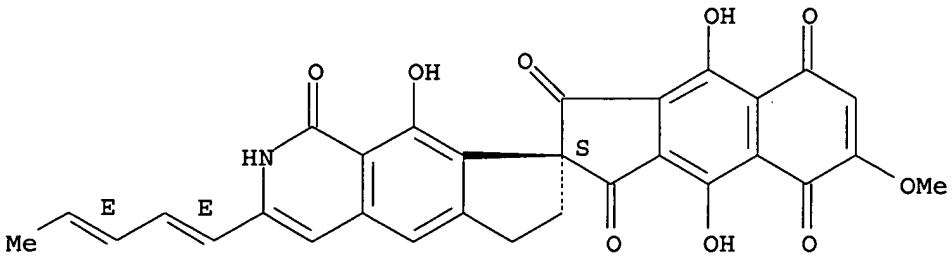
OS CASREACT 106:49879

IT **80455-68-1**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reduction and acetylation of)

RN 80455-68-1 CAPLUS

CN Spiro[2H-benz[f]indene-2,8'-[8H]cyclopent[g]isoquinoline]-1,1',3,5,8(2'H)-pentone, 6',7'-dihydro-4,9,9'-trihydroxy-6-methoxy-3'-[(1E,3E)-1,3-pentadienyl]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

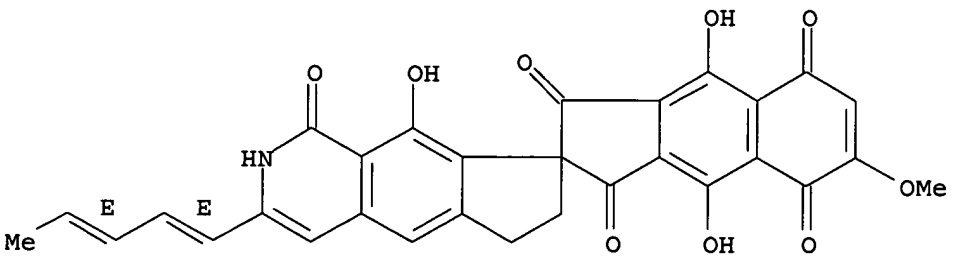


L8 ANSWER 104 OF 121 CAPLUS COPYRIGHT 2006 ACS on STN
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB (±)-Fredericamycin A (I) was prepared via the regiospecific, Me3Si-directed coupling of indane II with anhydride III to give the coupling product IV. Formation of the spiro system is achieved by reduction of IV to a keto aldehyde which undergoes in situ cyclization to the spiro ketols.
AN 1987:32665 CAPLUS
DN 106:32665
TI Synthesis of (±)-fredericamycin A
AU Kelly, T. Ross; Ohashi, Naohito; Armstrong-Chong, Rosemary J.; Bell, Stephen H.
CS Dep. Chem., Boston Coll., Chestnut Hill, MA, 02167, USA
SO Journal of the American Chemical Society (1986), 108(22), 7100-1
CODEN: JACSAT; ISSN: 0002-7863
DT Journal
LA English
OS CASREACT 106:32665
IT **104438-52-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(total synthesis of)
RN 104438-52-0 CAPLUS
CN Spiro[2H-benz[f]indene-2,8'-[8H]cyclopent[g]isoquinoline]-1,1',3,5,8(2'H)-pentone, 6',7'-dihydro-4,9,9'-trihydroxy-6-methoxy-3'-(1E,3E)-1,3-pentadienyl- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



L8 ANSWER 105 OF 121 CAPLUS COPYRIGHT 2006 ACS on STN

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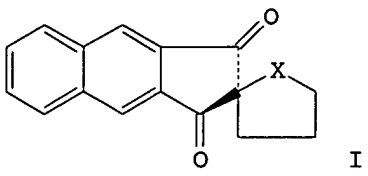


I

AB The 3 contiguous rings in the naphthalene portion of the model compds. I (X = CH2CH2, o-C6H4) related to Fredericamycin A have been prepared by the Diels-Alder cycloaddn. reaction of an α-bromo-o-quinodimethane intermediate to the C-C double bond of spiro[4.4]non-2-ene-1,4-dione.

AN 1986:626134 CAPLUS

DN 105:226134

TI Model studies aimed at the synthesis of fredericamycin A. A simple o-quinodimethane route to the spiro naphthalene portion

AU Bach, Robert D.; Klix, Russell C.

CS Dep. Chem., Wayne State Univ., Detroit, MI, 48202, USA

SO Tetrahedron Letters (1986), 27(18), 1983-6
CODEN: TELEAY; ISSN: 0040-4039

DT Journal

LA English

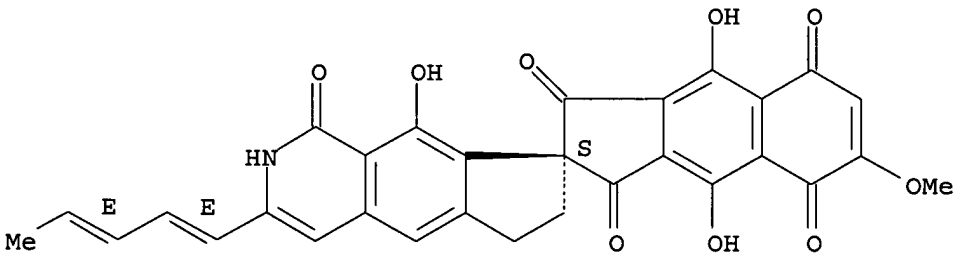
OS CASREACT 105:226134

IT **80455-68-1**
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclopentanaphthalenedione fragment of, model compound for)

RN 80455-68-1 CAPLUS

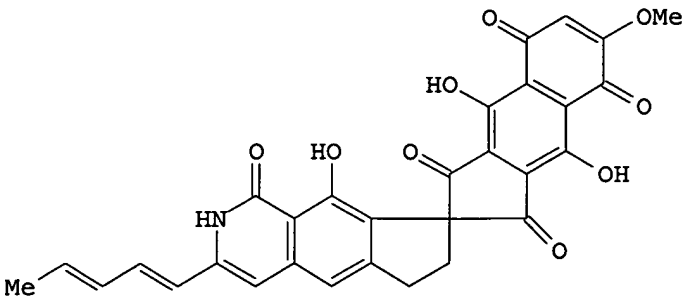
CN Spiro[2H-benz[f]indene-2,8'-[8H]cyclopent[g]isoquinoline]-1,1',3,5,8(2'H)-pentone, 6',7'-dihydro-4,9,9'-trihydroxy-6-methoxy-3'-[(1E,3E)-1,3-pentadienyl]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



L8 ANSWER 106 OF 121 CAPLUS COPYRIGHT 2006 ACS on STN

GI



I

AB NSC 305263 (fredericamycin A)(I) [**80455-68-1**], a newly described potent antitumor antibiotic, exhibits peculiar spectroscopic and phys. properties. The drug shows a striking color change from red to blue on exposure to O, with the appearance of an optical absorption band at 675 nm; on addition of acid, these changes are readily reversed. 1H and 13C NMR spectra of I show that the resonances from the quininoid half of the mol. disappear after exposure to O but reappear on acidification in parallel with the observed optical spectrum shift. These unusual NMR data are explained by ESR studies which demonstrate that I spontaneously forms an oxidized free radical with electron transfer to O. The observed hyperfine structure of this radical is consistent with 1-electron oxidation of the quininoid group. After I is exposed to O, an EPR signal is observed with axial symmetry with temperature and power saturation behavior suggestive of •O2-.

Spin-trapping EPR studies demonstrate that the drug reduces O to •O2- and H2O2 to •OH. This spontaneous mechanism of O reduction with the generation of oxidized drug free-radicals and reduced O free-radicals is unprecedented among anticancer drugs, suggesting that I could be the forerunner of a new class of anticancer drug.

AN 1986:545762 CAPLUS

DN 105:145762

TI Magnetic resonance studies of fredericamycin A: evidence for oxygen-dependent free-radical formation

AU Hilton, Bruce D.; Misra, Renuka; Zweier, Jay L.

CS Frederick Cancer Res. Facil., Natl. Cancer Inst., Frederick, MD, 21701, USA

SO Biochemistry (1986), 25(19), 5533-9
CODEN: BICHAW; ISSN: 0006-2960

DT Journal

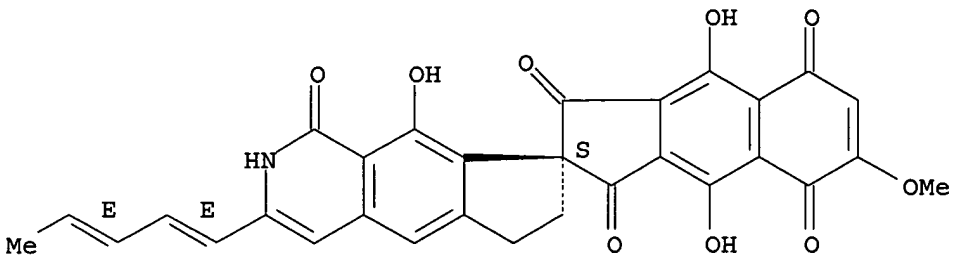
LA English

IT **80455-68-1**
RL: BIOL (Biological study)
(oxygen-dependent free-radical formation by, magnetic resonance study of)

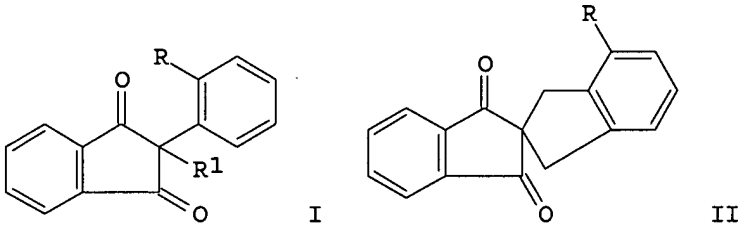
RN 80455-68-1 CAPLUS

CN Spiro[2H-benz[f]indene-2,8'-[8H]cyclopent[g]isoquinoline]-1,1',3,5,8(2'H)-pentone, 6',7'-dihydro-4,9,9'-trihydroxy-6-methoxy-3'-[(1E,3E)-1,3-pentadienyl]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



L8 ANSWER 107 OF 121 CAPLUS COPYRIGHT 2006 ACS on STN
GI

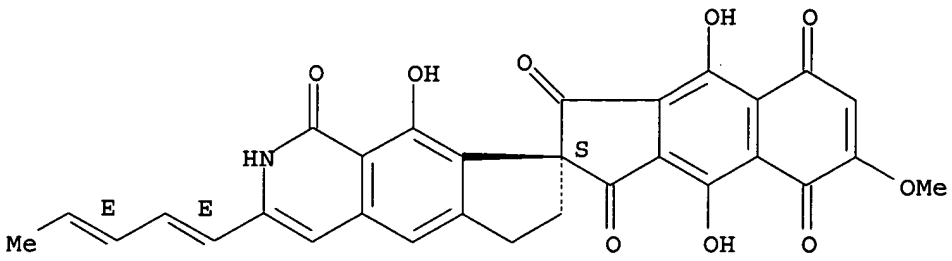


I II

AB An intramol. Friedel-Crafts type reaction of the thioacetals I [R = H, OMe, R1 = CH2CH(SEt)2], prepared from I (R1 = H) by allylation, ozonization, and reaction with EtSH, is the key step in a simple synthesis of the diketones II, which are model compds. for fredericamycin A.

AN 1986:514790 CAPLUS
DN 105:114790
TI Synthesis of spirocyclic diketones related to fredericamycin A
AU Braun, Manfred; Veith, Reiner
CS Inst. Org. Chem., Univ. Duesseldorf, Duesseldorf, D-4000/1, Fed. Rep. Ger.
SO Tetrahedron Letters (1986), 27(2), 179-82
CODEN: TELEAY; ISSN: 0040-4039
DT Journal
LA English
OS CASREACT 105:114790
IT **80455-68-1**
RL: RCT (Reactant); RACT (Reactant or reagent)
(dibenzospirononanedione model compds. for, preparation of)
RN 80455-68-1 CAPLUS
CN Spiro[2H-benz[f]indene-2,8'-[8H]cyclopent[g]isoquinoline]-1,1',3,5,8(2'H)-pentone, 6',7'-dihydro-4,9,9'-trihydroxy-6-methoxy-3'-[(1E,3E)-1,3-pentadienyl]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



L8 ANSWER 108 OF 121 CAPLUS COPYRIGHT 2006 ACS on STN
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

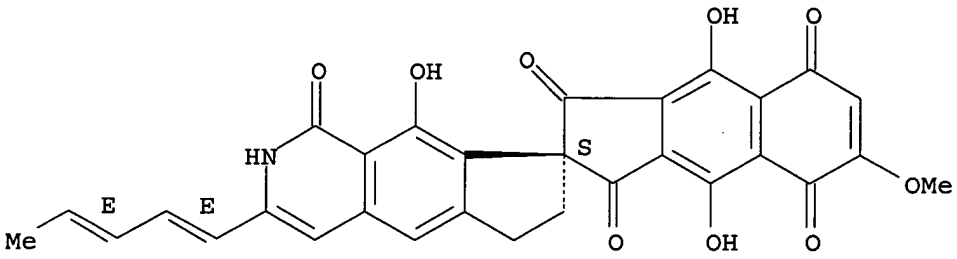
AB Stable fredericamycin A derivs. I and II (R = H, EtO2C, acyl; R1 = alkyl), useful as neoplasm inhibitors and bactericides, were prepared Thus, fredericamycin A (III, R = H)(IV) was treated with EtO2CCl in pyridine at 0° under stirring to give 83.% III (R = EtO2C), which was then treated with MeI and Ag2O in anhydrous dioxane at 75-80° under stirring to give 56.3% II (R = EtO2C, R1 = Me), whose i.p. administration prolonged the lives of mice transplanted with Ehrlich cancer cells (5 + 106 cells/animal) in a dose dependent manner. The title compds. also showed stronger antibacterial activities against Saccharomyces ruxii and Piricularia oryzae than IV in vitro.

AN 1986:497256 CAPLUS
DN 105:97256
TI Fredericamycin A derivatives
IN Hasegawa, Hiroshi; Yokoi, Koichi; Narita, Masa; Asaoka, Takemitsu; Kukita, Kenichi; Ishizeki, Seiji; Nakajima, Toshiaki
PA S. S. Pharmaceutical Co., Ltd., Japan
SO Jpn. Kokai Tokkyo Koho, 9 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 61044868	A2	19860304	JP 1984-166683	19840809
	JP 03031193	B4	19910502		
PRAI	JP 1984-166683		19840809		

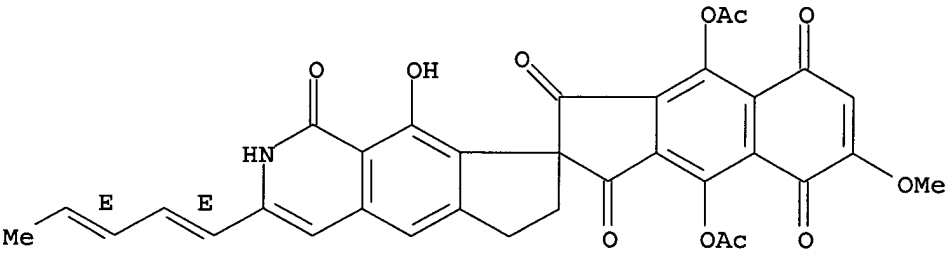
IT **80455-68-1**
RL: RCT (Reactant); RACT (Reactant or reagent)
(ethoxycarbonylation or reduction of)
RN 80455-68-1 CAPLUS
CN Spiro[2H-benz[f]indene-2,8'-[8H]cyclopent[g]isoquinoline]-1,1',3,5,8(2'H)-pentone, 6',7'-dihydro-4,9,9'-trihydroxy-6-methoxy-3'-[(1E,3E)-1,3-pentadienyl]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



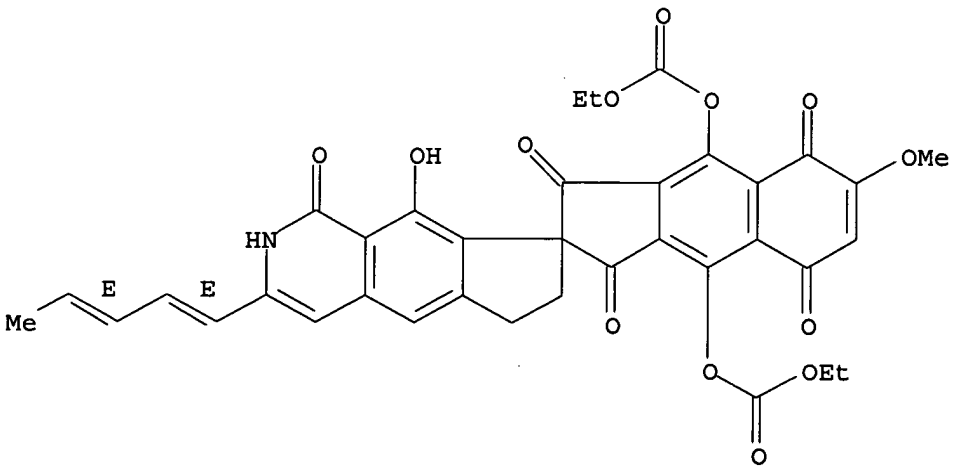
IT **97854-03-0P 103809-78-5P 103809-79-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and O-alkylation of)
RN 97854-03-0 CAPLUS
CN Spiro[2H-benz[f]indene-2,8'-[8H]cyclopent[g]isoquinoline]-1,1',3,5,8(2'H)-pentone, 4,9-bis(acetyloxy)-6',7'-dihydro-9'-hydroxy-6-methoxy-3'-(1,3-pentadienyl)-, (E,E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

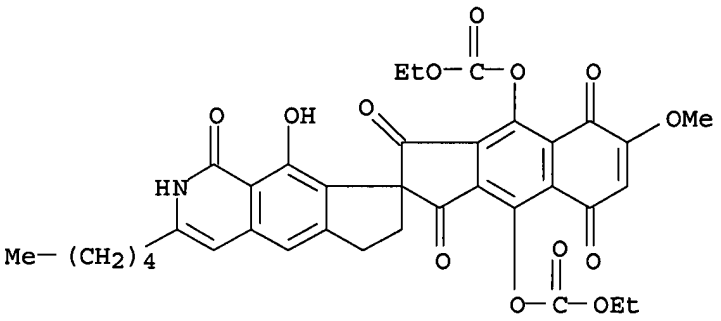


RN 103809-78-5 CAPLUS
CN Carbonic acid, 1,1',2',3,5,6',7',8-octahydro-9'-hydroxy-6-methoxy-1,1',3,5,8-pentaoxo-3'-(1,3-pentadienyl)spiro[2H-benz[f]indene-2,8'-[8H]cyclopent[g]isoquinoline]-4,9-diyl diethyl ester, (E,E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

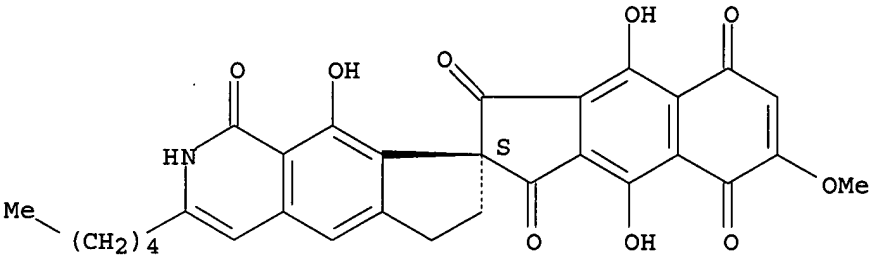


RN 103809-79-6 CAPLUS
CN Carbonic acid, 1,1',2',3,5,6',7',8-octahydro-9'-hydroxy-6-methoxy-1,1',3,5,8-pentaoxo-3'-pentylspiro[2H-benz[f]indene-2,8'-[8H]cyclopent[g]isoquinoline]-4,9-diyl diethyl ester (9CI) (CA INDEX NAME)



IT **97854-15-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and O-ethoxycarbonylation of)
RN 97854-15-4 CAPLUS
CN Spiro[2H-benz[f]indene-2,8'-[8H]cyclopent[g]isoquinoline]-1,1',3,5,8(2'H)-pentone, 6',7'-dihydro-4,9,9'-trihydroxy-6-methoxy-3'-pentyl-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L8 ANSWER 109 OF 121 CAPLUS COPYRIGHT 2006 ACS on STN
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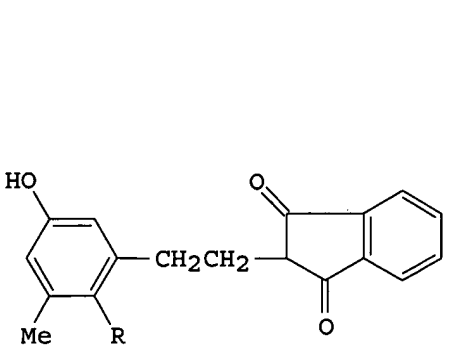
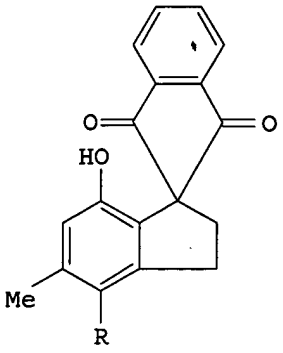
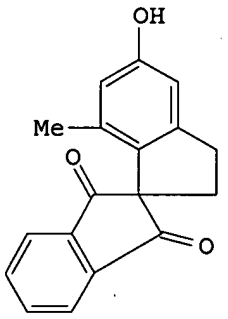


I



II



III

AB Ferricyanide oxidation of the phenolic β-diketones I (R = H, iodo) effects intramol. phenoxy-enoxy radical coupling to form the spiro systems II and III derived from C-C bond formation para or ortho to the phenolic O.

AN 1986:186201 CAPLUS

DN 104:186201

TI Synthesis of the spirocyclic center of fredericamycin A by phenoxy-enoxy radical coupling

AU Kende, Andrew S.; Ebetino, Frank H.; Ohta, Toshiharu

CS Dep. Chem., Univ. Rochester, Rochester, NY, 14627, USA

SO Tetrahedron Letters (1985), 26(26), 3063-6
CODEN: TELEAY; ISSN: 0040-4039

DT Journal

LA English

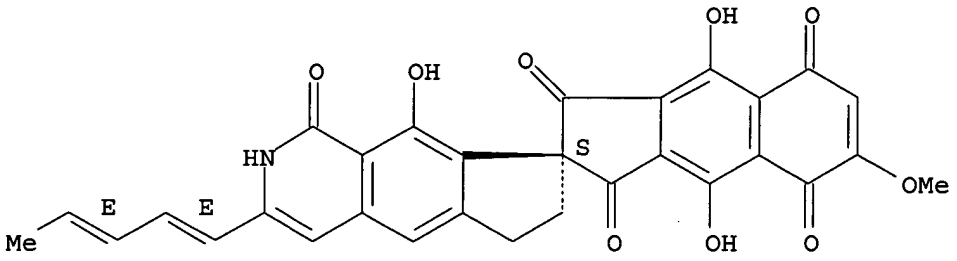
OS CASREACT 104:186201

IT **80455-68-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(spirobiindandione fragment of, preparation of)

RN 80455-68-1 CAPLUS

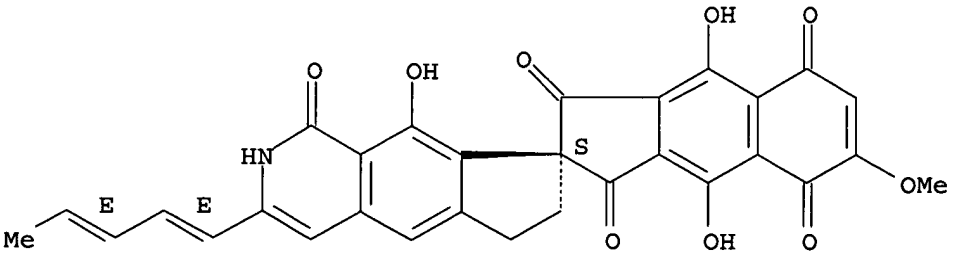
CN Spiro[2H-benz[f]indene-2,8'-[8H]cyclopent[g]isoquinoline]-1,1',3,5,8(2'H)-pentone, 6',7'-dihydro-4,9,9'-trihydroxy-6-methoxy-3'-[(1E,3E)-1,3-pentadienyl]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



L8 ANSWER 110 OF 121 CAPLUS COPYRIGHT 2006 ACS on STN
AB The title compound is monoclinic, space group P21/n, with a 12.544(2), b 7.507(1), c 13.480(2) Å, and β 97.09(1)°; dm = 1.312 and dc = 1.309 for Z = 4. Final R = 0.050 for 651 reflections. Atomic coordinates are given. The [4.4]nonane system is characteristic of fredericamycin A. The angle between the 2 aromatic portions at the spiro C (89.9(6)°) imposes the necessary spatial requirements and the C=O bond lengths (1.216(9) and 1.202(9) Å) indicate that they are property positioned for synthesis of fredericamycin A. The internal angles at the spiro C atom average 102.4(6)°.
AN 1986:178051 CAPLUS
DN 104:178051
TI Structure of 1,2'-spirobiindan-1',3'-dione, a key intermediate in the total synthesis of fredericamycin A
AU Acharya, K. R.; Puranik, Vedavati G.; Tavale, S. S.; Row, T. N. G.
CS Phys. Chem. Div., Natl. Chem. Lab., Pune, 411 008, India
SO Acta Crystallographica, Section C: Crystal Structure Communications (1986), C42(3), 334-6
CODEN: ACSCEE; ISSN: 0108-2701
DT Journal
LA English
IT **80455-68-1P**
RL: PREP (Preparation)
(structure of spirobiindandione as key intermediate in synthesis of)
RN 80455-68-1 CAPLUS
CN Spiro[2H-benz[f]indene-2,8'-[8H]cyclopent[g]isoquinoline]-1,1',3,5,8(2'H)-pentone, 6',7'-dihydro-4,9,9'-trihydroxy-6-methoxy-3'-[(1E,3E)-1,3-pentadienyl]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



L8 ANSWER 111 OF 121 CAPLUS COPYRIGHT 2006 ACS on STN
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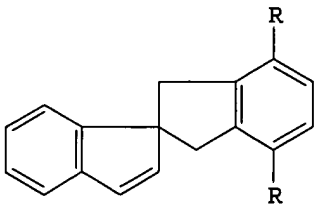
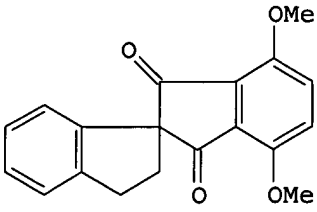


I



II

AB Indene was spiroalkylated with bis-1,2-bromomethylbenzene derivs. to give spiroindane I (R = H, OMe). Functionalization of the benzylic positions by acetoxylation, hydrolysis, and oxidation, after double bond reduction, led to the dihydroxydibenzospirononanedione ring system II of fredericamycin A.

AN 1986:168233 CAPLUS

DN 104:168233

TI Access to the spiro hydrindandione ring system of fredericamycin A through spiroalkylation and oxidation

AU Eck, G.; Julia, M.; Pfeiffer, B.; Rolando, C.

CS Lab. Chim., Ec. Norm. Super., Paris, 75231, Fr.

SO Tetrahedron Letters (1985), 26(39), 4725-6
CODEN: TELEAY; ISSN: 0040-4039

DT Journal

LA English

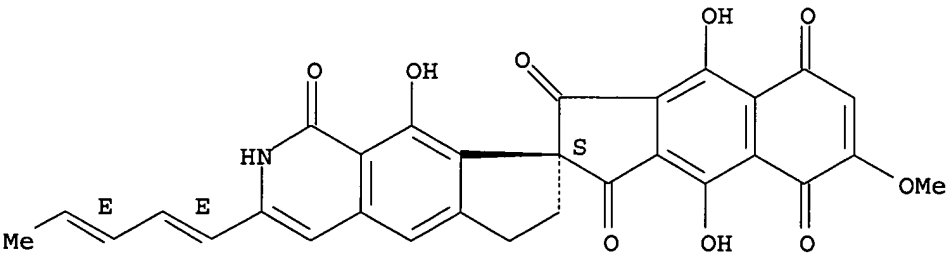
OS CASREACT 104:168233

IT **80455-68-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(dibenzospirononanedione fragment of, preparation of)

RN 80455-68-1 CAPLUS

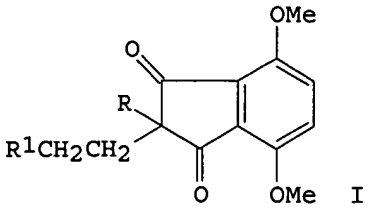
CN Spiro[2H-benz[f]indene-2,8'-[8H]cyclopent[g]isoquinoline]-1,1',3,5,8(2'H)-pentone, 6',7'-dihydro-4,9,9'-trihydroxy-6-methoxy-3'-[(1E,3E)-1,3-pentadienyl]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



L8 ANSWER 112 OF 121 CAPLUS COPYRIGHT 2006 ACS on STN

GI



I

AB Condensation of p-(MeO)2C6H4 with 1,1-cyclopentanedicarboxylic acid or 1,1-indanedicarboxylic acid derivs. led to the title compds. I (RR1 = CH2CH2, o-C6H4).

AN 1986:168232 CAPLUS

DN 104:168232

TI Access to the spiro hydrindandione ring system of fredericamycin A through a Friedel-Crafts reaction

AU Eck, G.; Julia, M.; Pfeiffer, B.; Rolando, C.

CS Lab. Chim., Ec. Norm. Super., Paris, 75231, Fr.

SO Tetrahedron Letters (1985), 26(39), 4723-4
CODEN: TELEAY; ISSN: 0040-4039

DT Journal

LA English

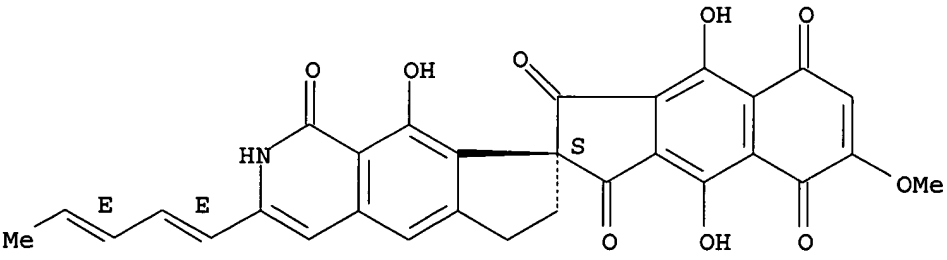
OS CASREACT 104:168232

IT **80455-68-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(hydrindandione fragment of, preparation of)

RN 80455-68-1 CAPLUS

CN Spiro[2H-benz[f]indene-2,8'-[8H]cyclopent[g]isoquinoline]-1,1',3,5,8(2'H)-pentone, 6',7'-dihydro-4,9,9'-trihydroxy-6-methoxy-3'-[(1E,3E)-1,3-pentadienyl]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



L8 ANSWER 113 OF 121 CAPLUS COPYRIGHT 2006 ACS on STN

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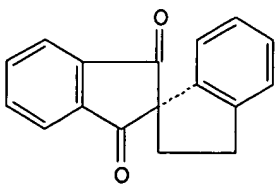
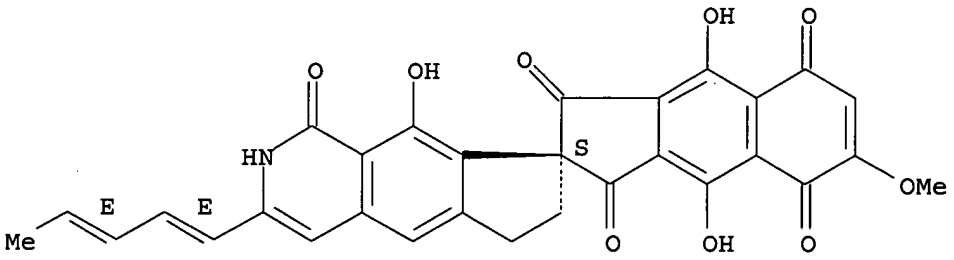


I

AB A synthesis involving the title reactions was developed for spiro compound I, a model compound for development of a synthetic route to fredericamycin A.
AN 1986:109320 CAPLUS
DN 104:109320
TI A mercury-mediated acyl migration in a pinacol-type rearrangement. Model studies toward the synthesis of fredericamycin A
AU Bach, Robert D.; Klix, Russell C.
CS Dep. Chem., Wayne State Univ., Detroit, MI, 48202, USA
SO Journal of Organic Chemistry (1986), 51(5), 749-52
CODEN: JOCEAH; ISSN: 0022-3263
DT Journal
LA English
OS CASREACT 104:109320
IT **80455-68-1**
RL: RCT (Reactant); RACT (Reactant or reagent)
(synthetic approach toward, model compds. for)
RN 80455-68-1 CAPLUS
CN Spiro[2H-benz[f]indene-2,8'-[8H]cyclopent[g]isoquinoline]-1,1',3,5,8(2'H)-pentone, 6',7'-dihydro-4,9,9'-trihydroxy-6-methoxy-3'-[(1E,3E)-1,3-pentadienyl]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

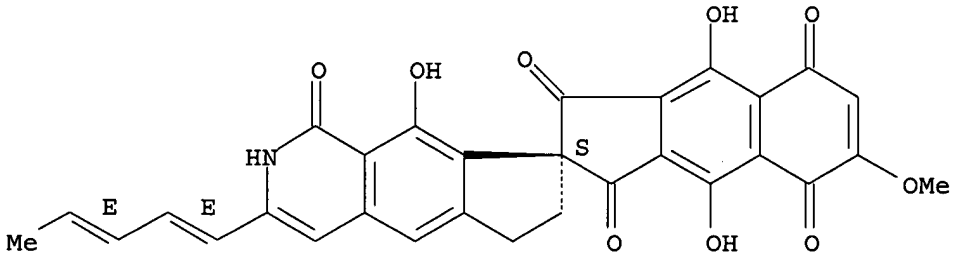


L8 ANSWER 114 OF 121 CAPLUS COPYRIGHT 2006 ACS on STN
GI For diagram(s), see printed CA Issue.
AB Title compds. I (R = acyl, X = Q, Q1), useful as neoplasm inhibitors (no data), were prepared Thus, fredericamycin A was reduced with H2 in THF in the presence of 10% Pd/C to give 60% tetrahydrofredericamycin A, which was treated with n-lauric anhydride in pyridine to give 75.6% I (R = n-lauroyl, X = Q).
AN 1986:33948 CAPLUS
DN 104:33948
TI Fredericamycin A derivatives
IN Yokoi, Koichi; Hasegawa, Hiroshi; Narita, Masa; Asaoka, Takemitsu; Kukita, Kenichi; Ishizeki, Seiji; Nakajima, Toshiaki
PA S. S. Pharmaceutical Co., Ltd., Japan
SO Jpn. Kokai Tokkyo Koho, 6 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 60152468	A2	19850810	JP 1984-6746	19840118

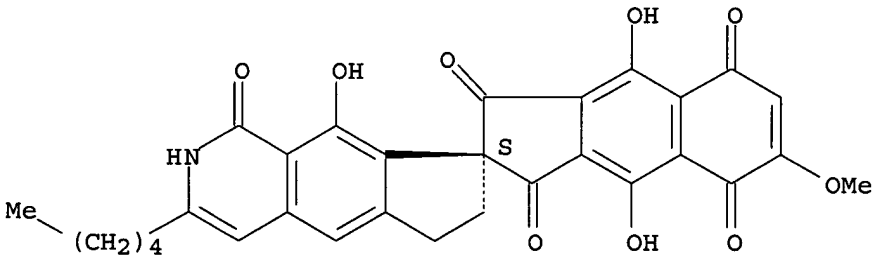
PRAI JP 1984-6746 19840118
OS CASREACT 104:33948
IT **80455-68-1**
RL: RCT (Reactant); RACT (Reactant or reagent)
(catalytic reduction of)
RN 80455-68-1 CAPLUS
CN Spiro[2H-benz[f]indene-2,8'-[8H]cyclopent[g]isoquinoline]-1,1',3,5,8(2'H)-pentone, 6',7'-dihydro-4,9,9'-trihydroxy-6-methoxy-3'-[(1E,3E)-1,3-pentadienyl]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

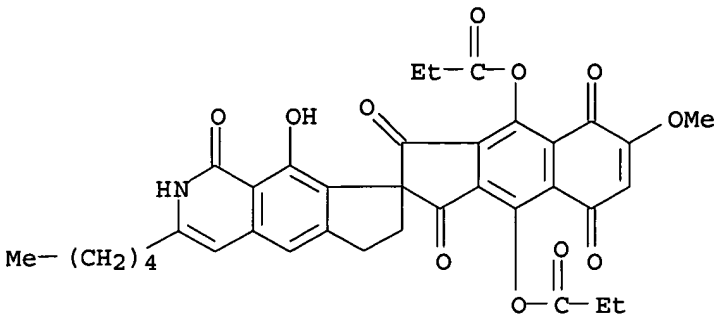


IT **97854-15-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and acylation of, by carboxylic anhydrides)
RN 97854-15-4 CAPLUS
CN Spiro[2H-benz[f]indene-2,8'-[8H]cyclopent[g]isoquinoline]-1,1',3,5,8(2'H)-pentone, 6',7'-dihydro-4,9,9'-trihydroxy-6-methoxy-3'-pentyl-, (2S)- (9CI) (CA INDEX NAME)

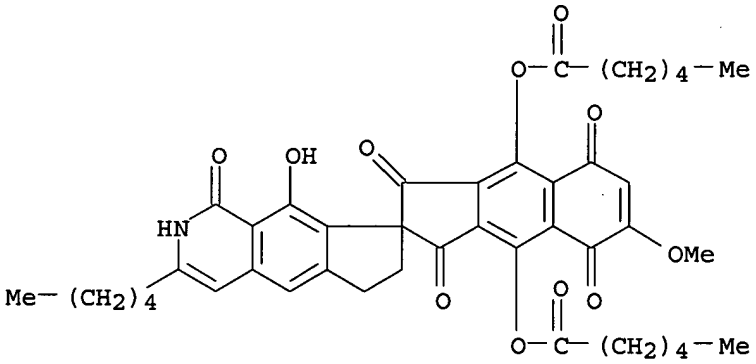
Absolute stereochemistry.



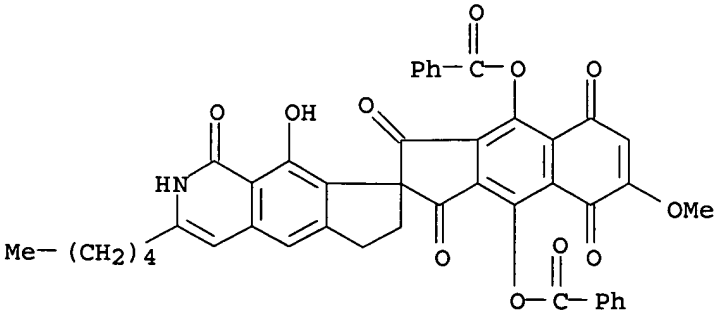
IT **97854-17-6P 97854-18-7P 97854-20-1P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of, as neoplasm inhibitor)
RN 97854-17-6 CAPLUS
CN Spiro[2H-benz[f]indene-2,8'-[8H]cyclopent[g]isoquinoline]-1,1',3,5,8(2'H)-pentone, 6',7'-dihydro-9'-hydroxy-6-methoxy-4,9-bis(1-oxopropoxy)-3'-pentyl- (9CI) (CA INDEX NAME)



RN 97854-18-7 CAPLUS
CN Hexanoic acid, 1,1',2',3,5,6',7',8-octahydro-9'-hydroxy-6-methoxy-1,1',3,5,8-pentaoxo-3'-pentylspiro[2H-benz[f]indene-2,8'-[8H]cyclopent[g]isoquinoline]-4,9-diyl ester (9CI) (CA INDEX NAME)

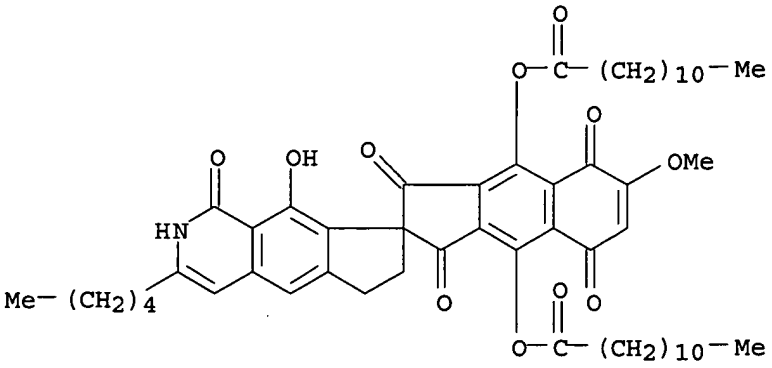


RN 97854-20-1 CAPLUS
CN Spiro[2H-benz[f]indene-2,8'-[8H]cyclopent[g]isoquinoline]-1,1',3,5,8(2'H)-pentone, 4,9-bis(benzoyloxy)-6',7'-dihydro-9'-hydroxy-6-methoxy-3'-pentyl- (9CI) (CA INDEX NAME)



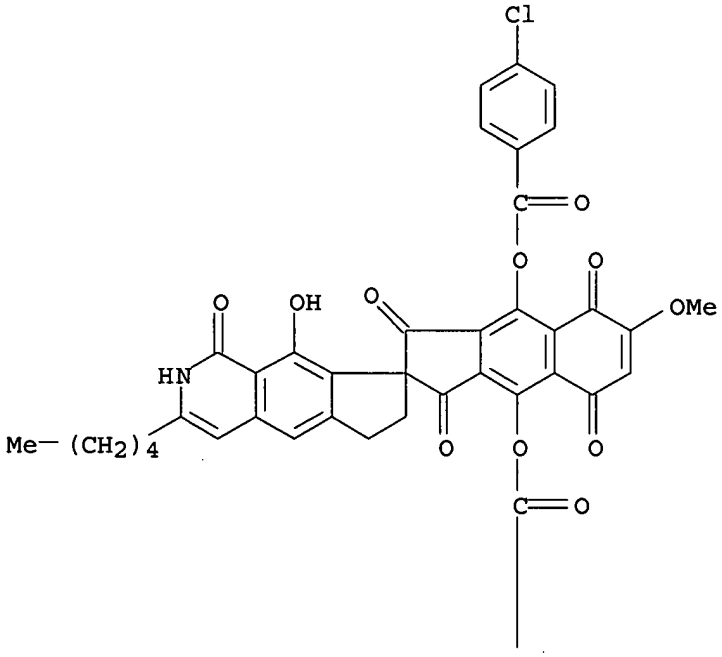
IT **97854-19-8P 97854-21-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as neoplasm inhibitors)
RN 97854-19-8 CAPLUS
CN Dodecanoic acid, 1,1',2',3,5,6',7',8-octahydro-9'-hydroxy-6-methoxy-1,1',3,5,8-pentaoxo-3'-pentylspiro[2H-benz[f]indene-2,8'-

[8H]cyclopent[g]isoquinoline]-4,9-diyl ester (9CI) (CA INDEX NAME)

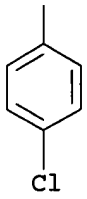


RN 97854-21-2 CAPLUS
CN Benzoic acid, 4-chloro-, 1,1',2',3,5,6',7',8-octahydro-9'-hydroxy-6-methoxy-1,1',3,5,8-pentaoxo-3'-pentylspiro[2H-benz[f]indene-2,8'-[8H]cyclopent[g]isoquinoline]-4,9-diyl ester (9CI) (CA INDEX NAME)

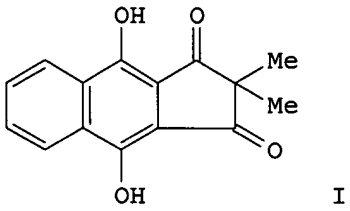
PAGE 1-A



PAGE 2-A



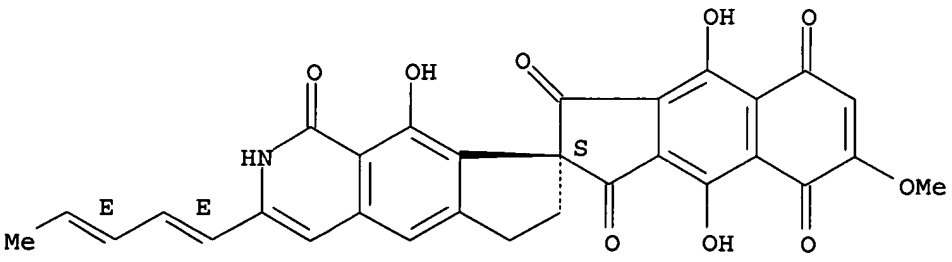
L8 ANSWER 115 OF 121 CAPLUS COPYRIGHT 2006 ACS on STN
GI



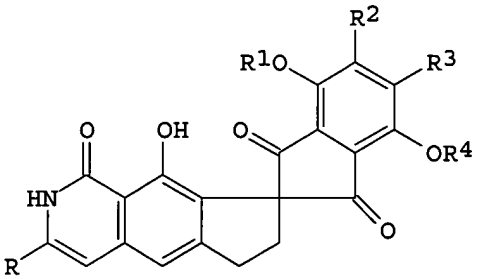
I

AB Benzindenedione I was prepared from 2,2-dimethyl-1,3-cyclopentanedione and 3-phenylsulfonylphthalide as a model for fredericamycin.
AN 1985:541693 CAPLUS
DN 103:141693
TI Synthesis of 2,2-disubstituted 4,9-dihydroxy-1H-benz[f]indene-1,3(2H)-diones. A model sequence for the synthesis of fredericamycin
AU Parker, Kathlyn A.; Koziski, Kathleen A.; Breault, Gloria
CS Dep. Chem., Brown Univ., Providence, RI, 02912, USA
SO Tetrahedron Letters (1985), 26(18), 2181-2
CODEN: TELEAY; ISSN: 0040-4039
DT Journal
LA English
OS CASREACT 103:141693
IT **80455-68-1**
RL: RCT (Reactant); RACT (Reactant or reagent)
(benzindenedione model compound for)
RN 80455-68-1 CAPLUS
CN Spiro[2H-benz[f]indene-2,8'-[8H]cyclopent[g]isoquinoline]-1,1',3,5,8(2'H)-pentone, 6',7'-dihydro-4,9,9'-trihydroxy-6-methoxy-3'-[(1E,3E)-1,3-pentadienyl]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



L8 ANSWER 116 OF 121 CAPLUS COPYRIGHT 2006 ACS on STN
GI



I

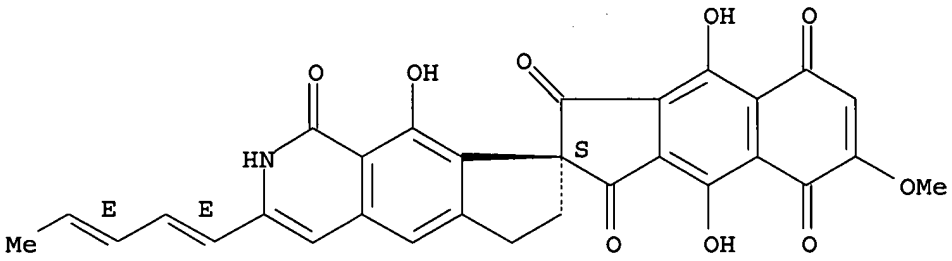
AB Fredericamycin A derivs. I [R = CH:CHCH:CHMe, pentyl; R1 = H, acyl; R2R3 = COCH:C(OMe)CO, C(OR1):CHC(OMe):COR1] were prepared Thus fredericamycin A (II) was acetylated to give I [R = CH:CHCH:CHMe, R1 = Ac, R2R3 = COCH:C(OMe)CO, III]. Catalytic hydrogenation of II, followed by acetylation, gave I [R = pentyl, R1 = Ac, R2R3 = C(OAc):CHC(OMe):COAc]. Catalytic hydrogenation of II, followed by treatment with Me2SO, gave I [R = pentyl, R1 = H, R2R3 = COCH:C(OMe)CO (IV, R1 = H)] which was acetylated to IV (R1 = Ac). III and IV (R1 = Ac) had min. inhibitory concns. against Staphylococcus aureus Smith of 6.25 and 25 μg/mL, resp. They had antitumor activity i.p. in mice at 0.125 and 4.0 mg/kg day.

AN 1985:504798 CAPLUS
DN 103:104798
TI Fredericamycin A derivative
IN Yokoi, Koichi; Hasegawa, Hiroshi; Narita, Tadashi; Asaoka, Takemitsu; Kurita, Kenichi; Ishizeki, Seiji; Nakashima, Toshiaki
PA S. S. Pharmaceutical Co., Ltd., Japan
SO Ger. Offen., 44 pp.
CODEN: GWXXBX
DT Patent
LA German
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 3430365	A1	19850307	DE 1984-3430365	19840817
	JP 60042368	A2	19850306	JP 1983-150522	19830818
	JP 01019386	B4	19890411		
	JP 60056960	A2	19850402	JP 1983-165489	19830908
	JP 01049267	B4	19891024		
	JP 60058964	A2	19850405	JP 1983-166082	19830909
	JP 01049268	B4	19891024		
	GB 2145084	A1	19850320	GB 1984-20246	19840809
	GB 2145084	B2	19870128		
	US 4584377	A	19860422	US 1984-639113	19840809
	CA 1267147	A1	19900327	CA 1984-460842	19840813
	FR 2550791	A1	19850222	FR 1984-12905	19840817
	FR 2550791	B1	19881014		
	CH 669379	A	19890315	CH 1984-3957	19840817
PRAI	JP 1983-150522	A	19830818		
	JP 1983-165489	A	19830908		

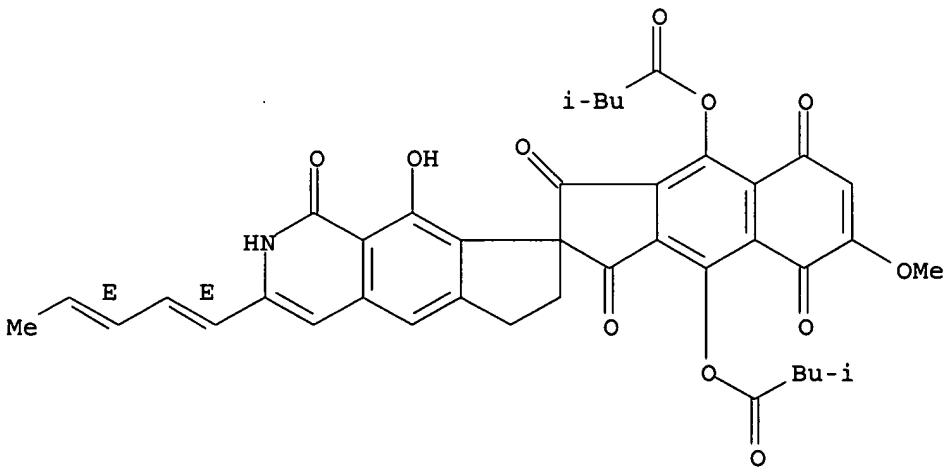
JP 1983-166082 A 19830909
OS CASREACT 103:104798; MARPAT 103:104798
IT **80455-68-1**
RL: RCT (Reactant); RACT (Reactant or reagent)
(acylation of)
RN 80455-68-1 CAPLUS
CN Spiro[2H-benz[f]indene-2,8'-[8H]cyclopent[g]isoquinoline]-1,1',3,5,8(2'H)-pentone, 6',7'-dihydro-4,9,9'-trihydroxy-6-methoxy-3'-[(1E,3E)-1,3-pentadienyl]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



IT **97854-04-1P 97854-09-6P 97854-11-0P**
97867-35-1P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and antitumor activity of)
RN 97854-04-1 CAPLUS
CN Butanoic acid, 3-methyl-, 1,1',2',3,5,6',7',8-octahydro-9'-hydroxy-6-methoxy-1,1',3,5,8-pentaoxo-3'-(1,3-pentadienyl)spiro[2H-benz[f]indene-2,8'-[8H]cyclopent[g]isoquinoline]-4,9-diyl ester, (E,E)- (9CI) (CA INDEX NAME)

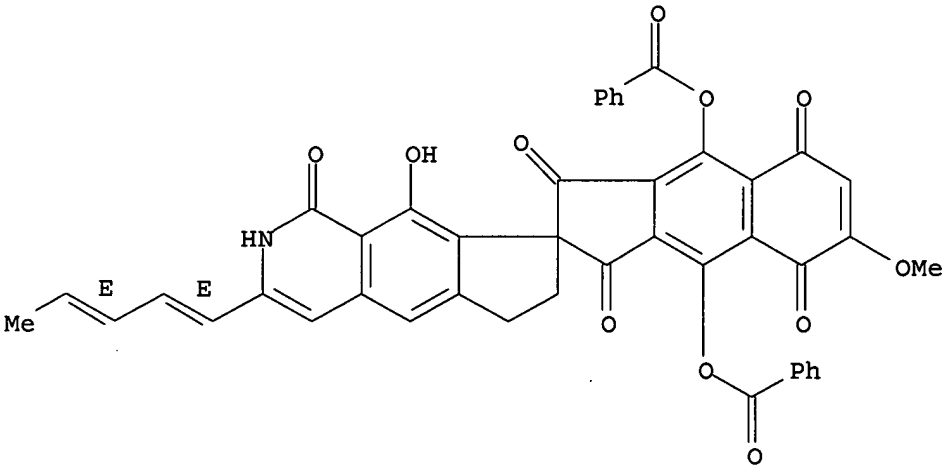
Double bond geometry as shown.



RN 97854-09-6 CAPLUS
CN Spiro[2H-benz[f]indene-2,8'-[8H]cyclopent[g]isoquinoline]-1,1',3,5,8(2'H)-pentone, 4,9-bis(benzoyloxy)-6',7'-dihydro-9'-hydroxy-6-methoxy-3'-(1,3-

pentadienyl)-, (E,E)- (9CI) (CA INDEX NAME)

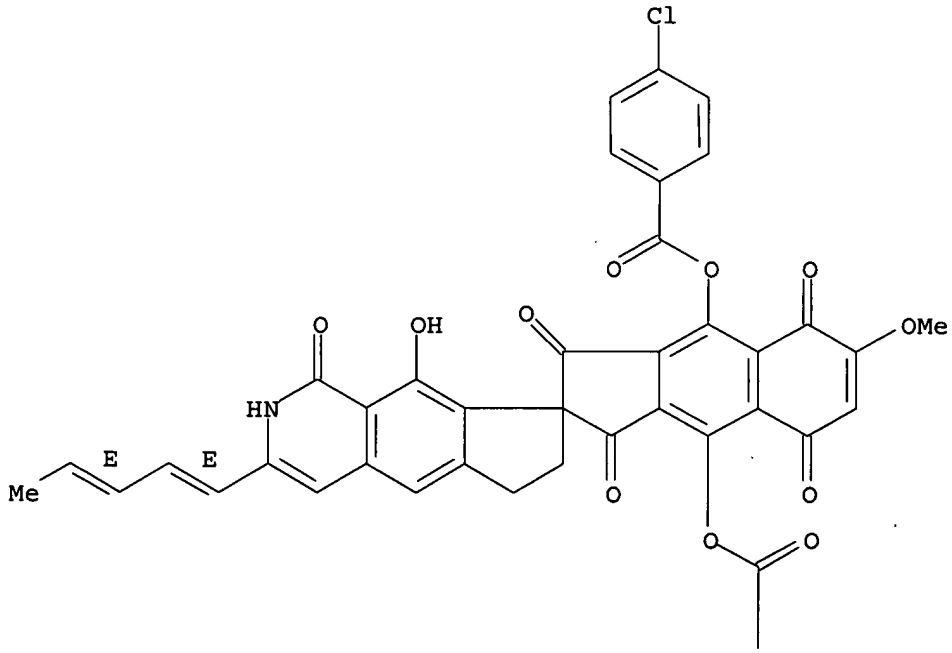
Double bond geometry as shown.



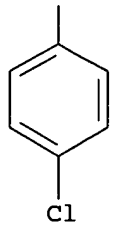
RN 97854-11-0 CAPLUS
CN Benzoic acid, 4-chloro-, 1,1',2',3,5,6',7',8-octahydro-9'-hydroxy-6-methoxy-1,1',3,5,8-pentaoxo-3'-(1,3-pentadienyl)spiro[2H-benz[f]indene-2,8'-[8H]cyclopent[g]isoquinoline]-4,9-diyl ester, (E,E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A

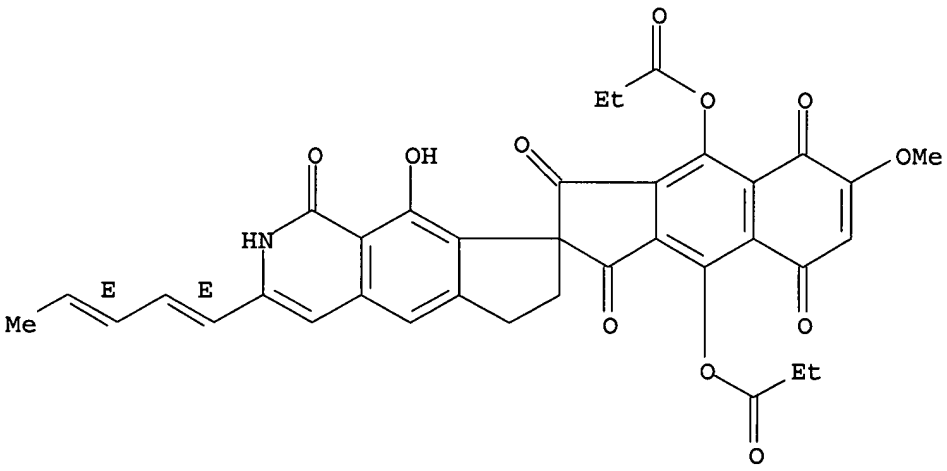


PAGE 2-A



RN 97867-35-1 CAPLUS
CN Spiro[2H-benz[f]indene-2,8'-[8H]cyclopent[g]isoquinoline]-1,1',3,5,8(2'H)-pentone, 6',7'-dihydro-9'-hydroxy-6-methoxy-4,9-bis(1-oxopropoxy)-3'-(1,3-pentadienyl)-, (E,E)- (9CI) (CA INDEX NAME)

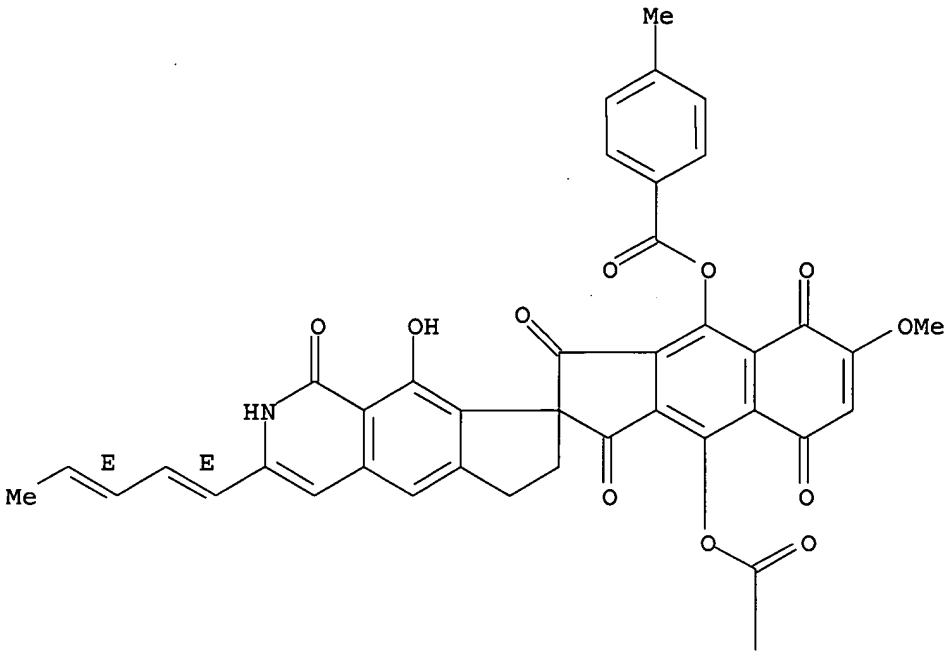
Double bond geometry as shown.



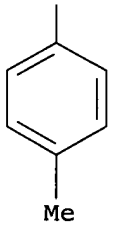
IT **97854-05-2P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and bactericidal and fungicidal activity of)
RN 97854-05-2 CAPLUS
CN Benzoic acid, 4-methyl-, 1,1',2',3,5,6',7',8-octahydro-9'-hydroxy-6-methoxy-1,1',3,5,8-pentaoxo-3'-(1,3-pentadienyl)spiro[2H-benz[f]indene-2,8'-[8H]cyclopent[g]isoquinoline]-4,9-diyl ester, (E,E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A

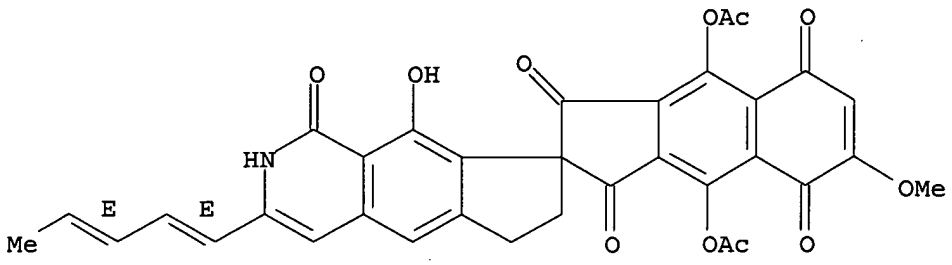


PAGE 2-A



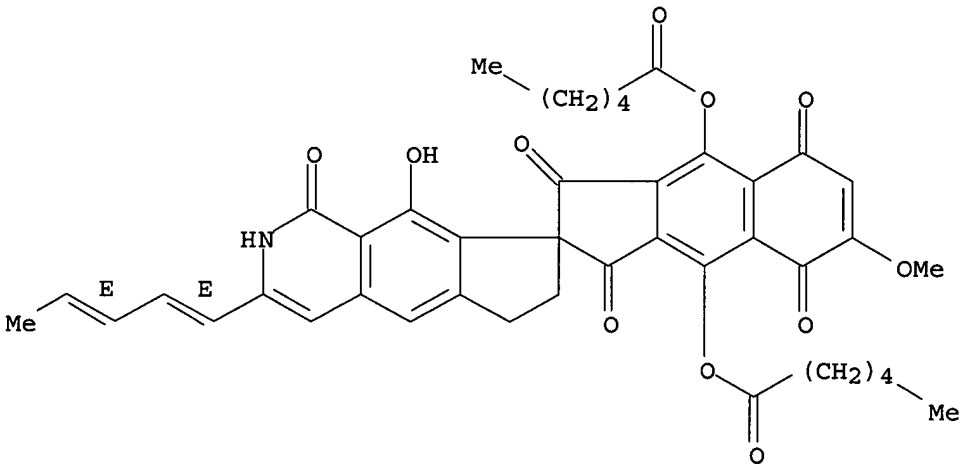
IT **97854-03-0P 97854-06-3P 97854-08-5P**
97854-10-9P 97854-16-5P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and bactericidal, fungicidal, and antitumor activity of)
RN 97854-03-0 CAPLUS
CN Spiro[2H-benz[f]indene-2,8'-[8H]cyclopent[g]isoquinoline]-1,1',3,5,8(2'H)-pentone, 4,9-bis(acetyloxy)-6',7'-dihydro-9'-hydroxy-6-methoxy-3'-(1,3-pentadienyl)-, (E,E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



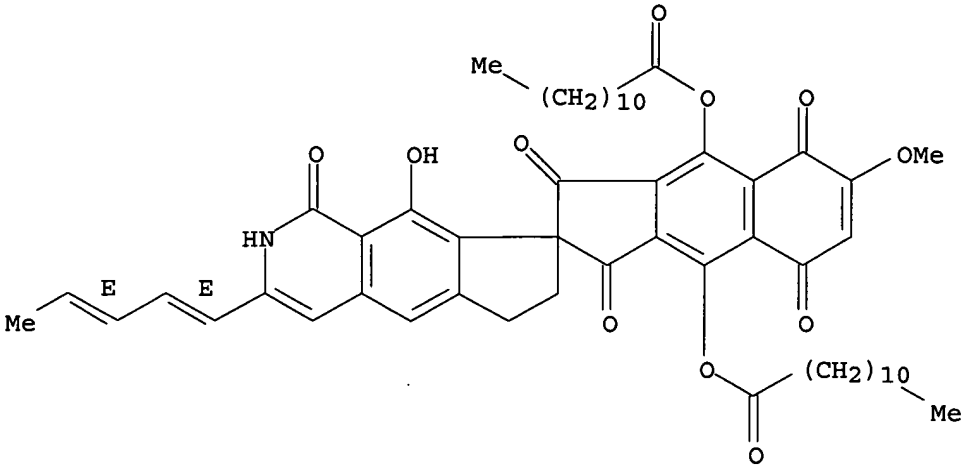
RN 97854-06-3 CAPLUS
CN Hexanoic acid, 1,1',2',3,5,6',7',8-octahydro-9'-hydroxy-6-methoxy-1,1',3,5,8-pentaoxo-3'-(1,3-pentadienyl)spiro[2H-benz[f]indene-2,8'-[8H]cyclopent[g]isoquinoline]-4,9-diyl ester, (E,E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 97854-08-5 CAPLUS
CN Dodecanoic acid, 1,1',2',3,5,6',7',8-octahydro-9'-hydroxy-6-methoxy-1,1',3,5,8-pentaoxo-3'-(1,3-pentadienyl)spiro[2H-benz[f]indene-2,8'-[8H]cyclopent[g]isoquinoline]-4,9-diyl ester, (E,E)- (9CI) (CA INDEX NAME)

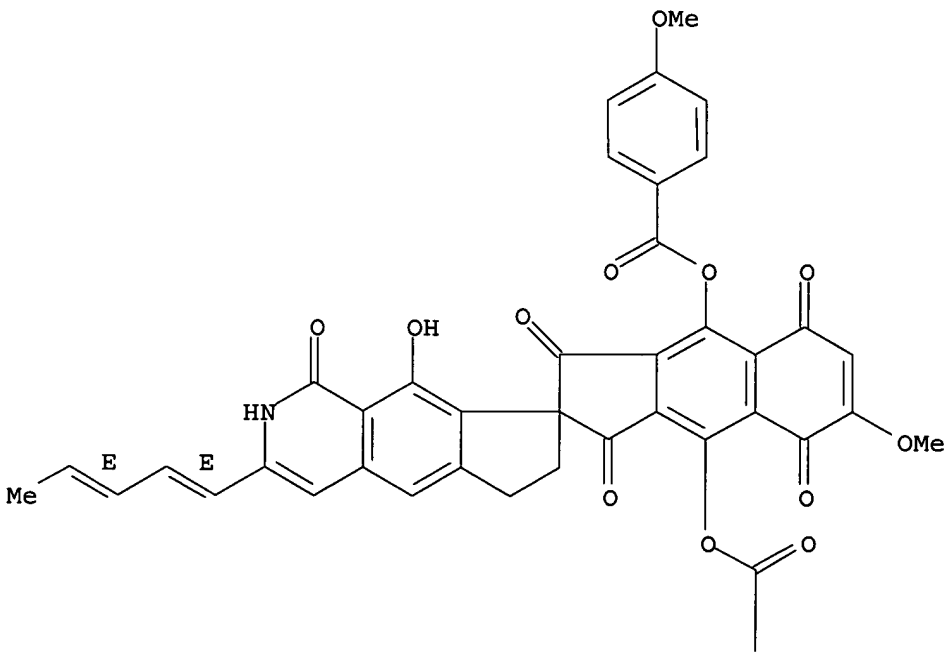
Double bond geometry as shown.



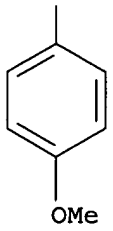
RN 97854-10-9 CAPLUS
CN Benzoic acid, 4-methoxy-, 1,1',2',3,5,6',7',8-octahydro-9'-hydroxy-6-methoxy-1,1',3,5,8-pentaoxo-3'-(1,3-pentadienyl)spiro[2H-benz[f]indene-2,8'-[8H]cyclopent[g]isoquinoline]-4,9-diyl ester, (E,E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

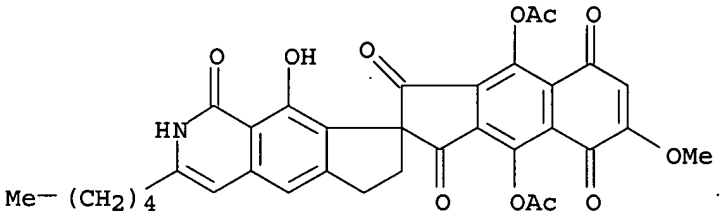
PAGE 1-A



PAGE 2-A

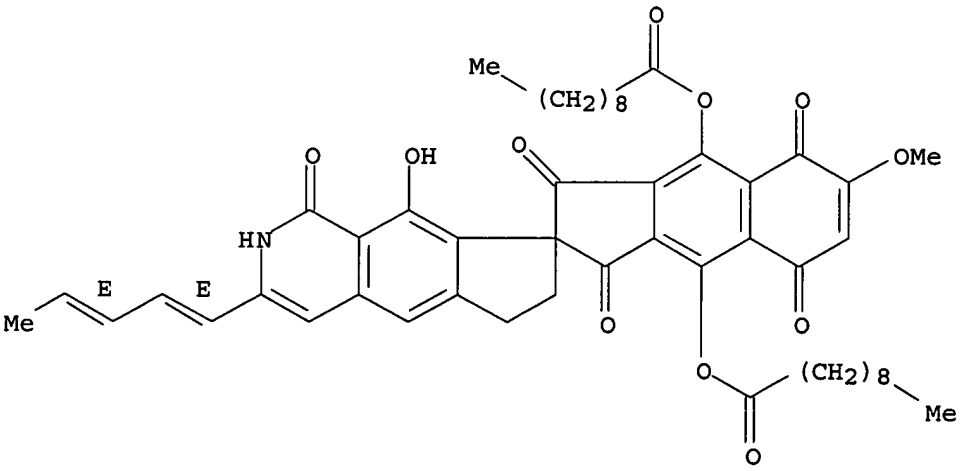


RN 97854-16-5 CAPLUS
CN Spiro[2H-benz[f]indene-2,8'-[8H]cyclopent[g]isoquinoline]-1,1',3,5,8(2'H)-pentone, 4,9-bis(acetyloxy)-6',7'-dihydro-9'-hydroxy-6-methoxy-3'-pentyl- (9CI) (CA INDEX NAME)

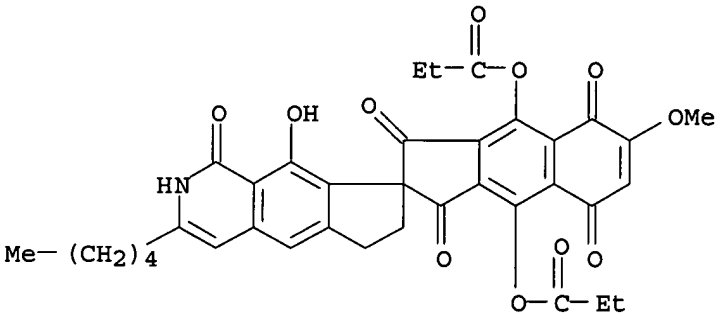


IT **97854-07-4P 97854-17-6P 97854-18-7P 97854-19-8P 97854-20-1P 97854-21-2P 97867-36-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 97854-07-4 CAPLUS
CN Decanoic acid, 1,1',2',3,5,6',7',8-octahydro-9'-hydroxy-6-methoxy-1,1',3,5,8-pentaoxo-3'-(1,3-pentadienyl)spiro[2H-benz[f]indene-2,8'-[8H]cyclopent[g]isoquinoline]-4,9-diyl ester, (E,E)- (9CI) (CA INDEX NAME)

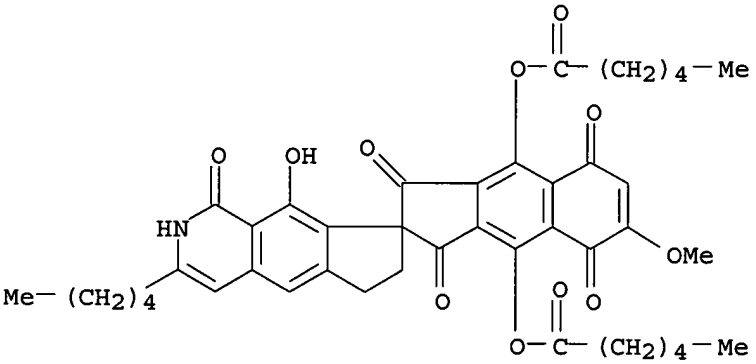
Double bond geometry as shown.



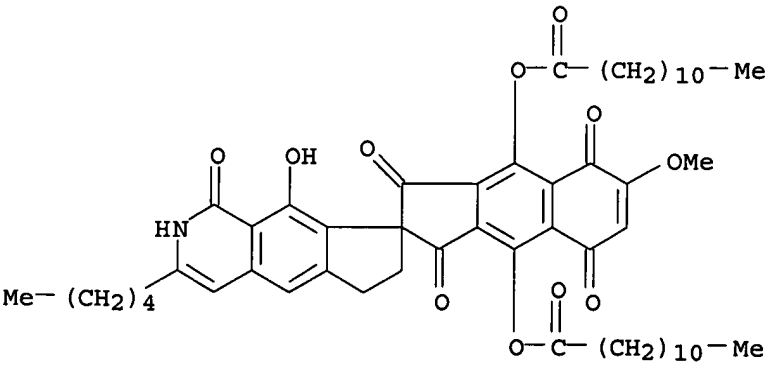
RN 97854-17-6 CAPLUS
CN Spiro[2H-benz[f]indene-2,8'-[8H]cyclopent[g]isoquinoline]-1,1',3,5,8(2'H)-pentone, 6',7'-dihydro-9'-hydroxy-6-methoxy-4,9-bis(1-oxopropoxy)-3'-pentyl- (9CI) (CA INDEX NAME)



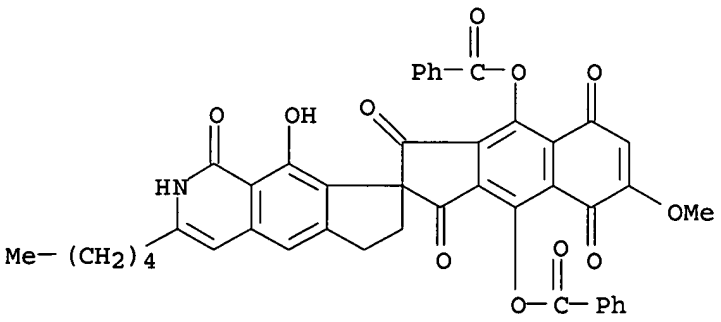
RN 97854-18-7 CAPLUS
CN Hexanoic acid, 1,1',2',3,5,6',7',8-octahydro-9'-hydroxy-6-methoxy-1,1',3,5,8-pentaoxo-3'-pentylspiro[2H-benz[f]indene-2,8'-[8H]cyclopent[g]isoquinoline]-4,9-diyl ester (9CI) (CA INDEX NAME)



RN 97854-19-8 CAPLUS
CN Dodecanoic acid, 1,1',2',3,5,6',7',8-octahydro-9'-hydroxy-6-methoxy-1,1',3,5,8-pentaoxo-3'-pentylspiro[2H-benz[f]indene-2,8'-[8H]cyclopent[g]isoquinoline]-4,9-diyl ester (9CI) (CA INDEX NAME)

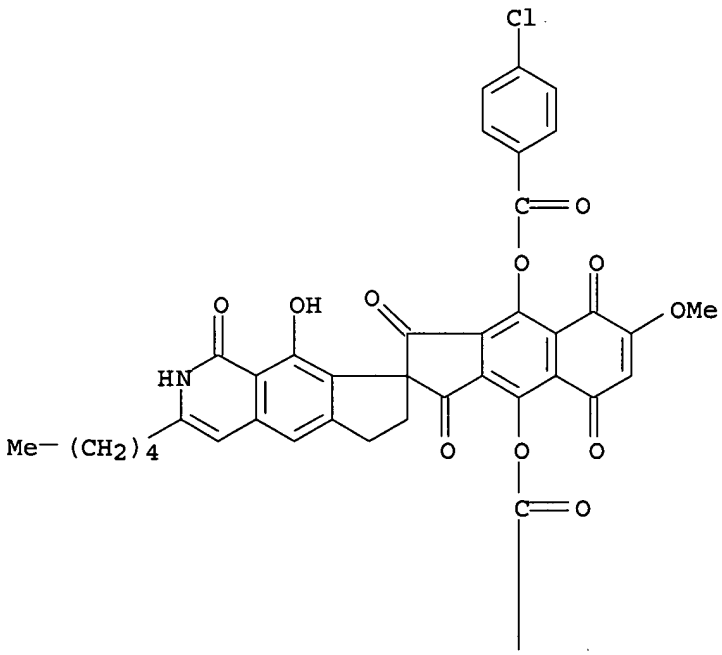


RN 97854-20-1 CAPLUS
CN Spiro[2H-benz[f]indene-2,8'-[8H]cyclopent[g]isoquinoline]-1,1',3,5,8(2'H)-pentone, 4,9-bis(benzoyloxy)-6',7'-dihydro-9'-hydroxy-6-methoxy-3'-pentyl- (9CI) (CA INDEX NAME)

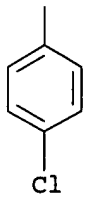


RN 97854-21-2 CAPLUS
CN Benzoic acid, 4-chloro-, 1,1',2',3,5,6',7',8-octahydro-9'-hydroxy-6-methoxy-1,1',3,5,8-pentaoxo-3'-pentylspiro[2H-benz[f]indene-2,8'-[8H]cyclopent[g]isoquinoline]-4,9-diyl ester (9CI) (CA INDEX NAME)

PAGE 1-A



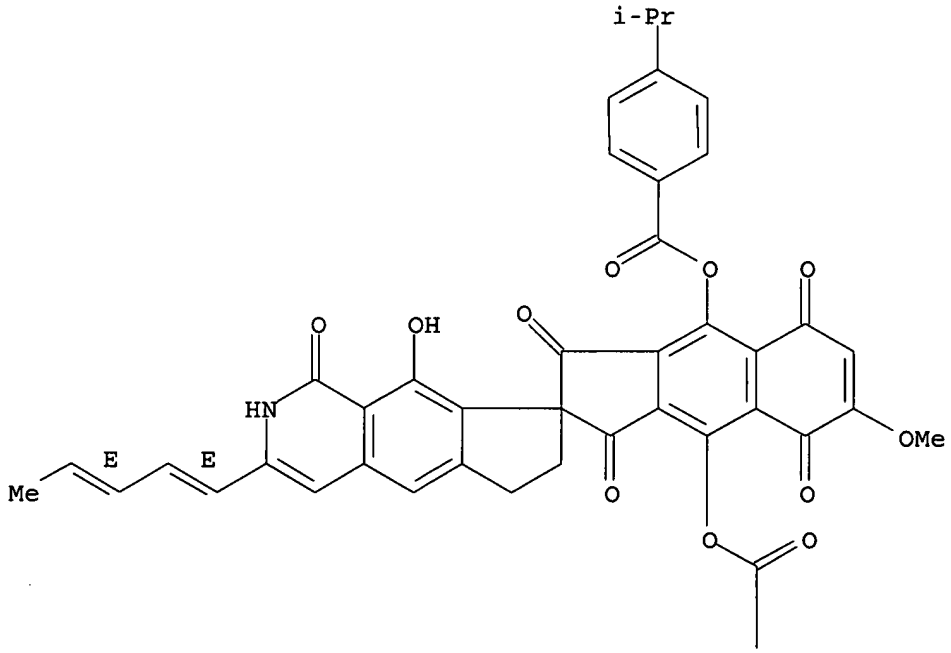
PAGE 2-A



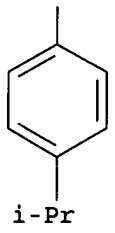
RN 97867-36-2 CAPLUS
CN Benzoic acid, 4-(1-methylethyl)-, 1,1',2',3,5,6',7',8-octahydro-9'-hydroxy-6-methoxy-1,1',3,5,8-pentaoxo-3'-(1,3-pentadienyl)spiro[2H-benz[f]indene-2,8'-[8H]cyclopent[g]isoquinoline-4,9-diyl] ester, (E,E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A

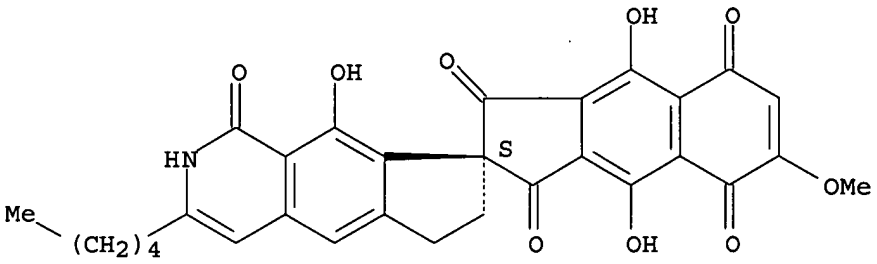


PAGE 2-A



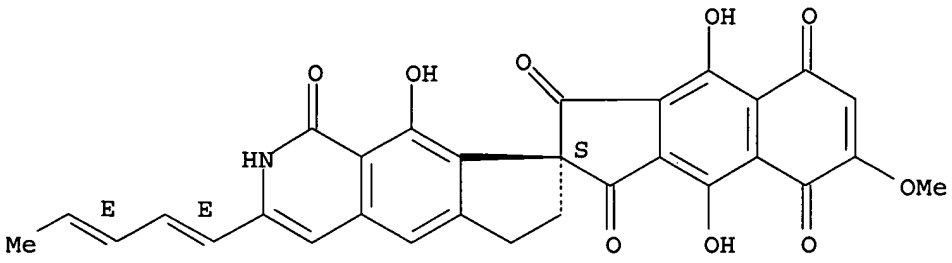
IT **97854-15-4P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(preparation, acylation, and antitumor activity of)
RN 97854-15-4 CAPLUS
CN Spiro[2H-benz[f]indene-2,8'-[8H]cyclopent[g]isoquinoline]-1,1',3,5,8(2'H)-pentone, 6',7'-dihydro-4,9,9'-trihydroxy-6-methoxy-3'-pentyl-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

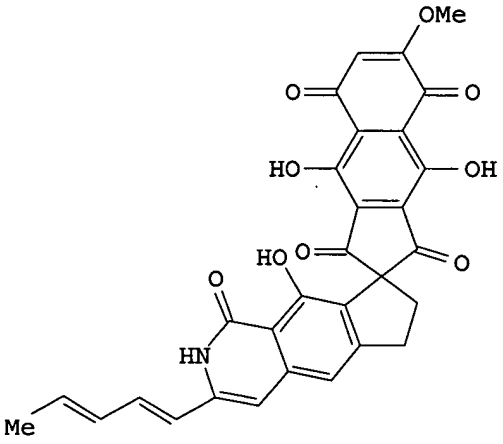


L8 ANSWER 117 OF 121 CAPLUS COPYRIGHT 2006 ACS on STN
GI For diagram(s), see printed CA Issue.
AB The spiro[4.4]nonane system I, present in fredericamycin A, was prepared by Dieckmann condensation of phthalide with 1-hydroxyisochroman, followed by cyclization of the hydroxy diketone II to the tetracycle III, and thermal isomerization of III to I. The structure of I was determined by x-ray crystallog.
AN 1985:95359 CAPLUS
DN 102:95359
TI Methodology for the synthesis of a spiro[4.4]nonane system: an approach for the total synthesis of fredericamycin A
AU Rao, A. V. Rama; Reddy, D. Reddeppa; Deshpande, V. H.
CS Natl. Chem. Lab., Poona City, 411008, India
SO Journal of the Chemical Society, Chemical Communications (1984), (16), 1119-20
CODEN: JCCCAT; ISSN: 0022-4936
DT Journal
LA English
IT **80455-68-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of spirononane moiety of)
RN 80455-68-1 CAPLUS
CN Spiro[2H-benz[f]indene-2,8'-[8H]cyclopent[g]isoquinoline]-1,1',3,5,8(2'H)-pentone, 6',7'-dihydro-4,9,9'-trihydroxy-6-methoxy-3'-[(1E,3E)-1,3-pentadienyl]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



L8 ANSWER 118 OF 121 CAPLUS COPYRIGHT 2006 ACS on STN
GI



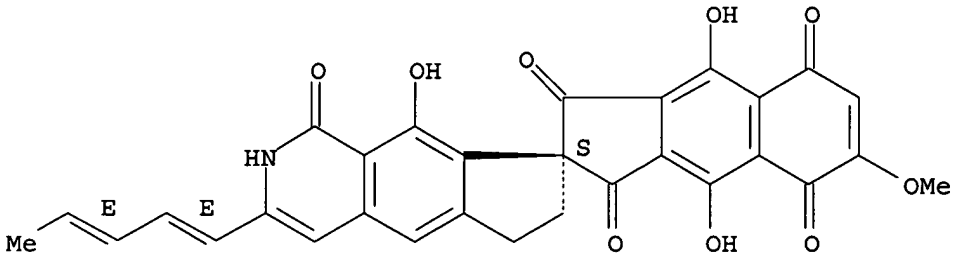
I

AB Fredericamycin A (I), produced by a strain of Streptomyces griseus, represents a new structural class of antitumor antibiotics containing a spiro ring system. Glucose in the fermentation medium was not utilized until late in the growth stage, just prior to synthesis of I. [14C]glucose tracer expts. demonstrated that glucose is incorporated into I by catabolism to acetate. Biosynthetic enrichment of I with single- and double-labeled [13C]acetate showed that the entire C-skeleton of the spiro ring system is derived from acetate. L-Methionine provided the only nonskeletal C in I, the methoxy C at position C-6. The direction of the polyketide chain and the position of the C lost during biosynthesis were established in using expts. with stable isotopes. A general model for I biosynthesis is proposed, and a possible scheme for the formation of the spiro C center is presented.

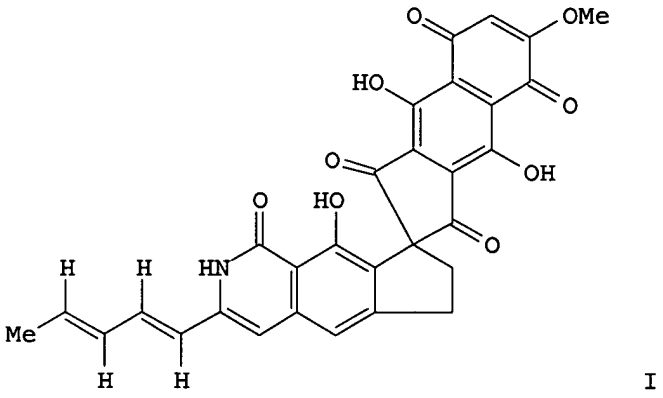
AN 1985:75415 CAPLUS
DN 102:75415
TI Biosynthesis of fredericamycin A, a new antitumor antibiotic
AU Byrne, Kevin M.; Hilton, Bruce D.; White, Richard J.; Misra, Renuka; Pandey, Ramesh C.
CS Program Resources, Inc., Frederick, MD, 21701, USA
SO Biochemistry (1985), 24(2), 478-86
CODEN: BICHAW; ISSN: 0006-2960
DT Journal

LA English
IT **80455-68-1**
RL: FORM (Formation, nonpreparative)
(formation of, pathway of)
RN 80455-68-1 CAPLUS
CN Spiro[2H-benz[f]indene-2,8'-[8H]cyclopent[g]isoquinoline]-1,1',3,5,8(2'H)-pentone, 6',7'-dihydro-4,9,9'-trihydroxy-6-methoxy-3'-[(1E,3E)-1,3-pentadienyl]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



L8 ANSWER 119 OF 121 CAPLUS COPYRIGHT 2006 ACS on STN
GI

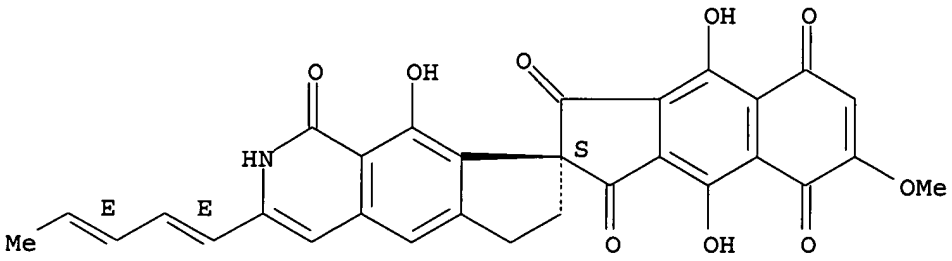


I

AB The structures of fredericamycin A (I), an antitumor antibiotic produced by Streptomyces griseus was confirmed by single crystal x-ray anal., together with the high-resolution electron impact, field desorption, and fast atom bombardment mass spectral and proton NMR studies. The structure has a novel spiro ring system, not previously found in the antibiotic structures.
AN 1982:472154 CAPLUS
DN 97:72154
TI Fredericamycin A, an antitumor antibiotic of a novel skeletal type
AU Misra, Renuka; Pandey, Ramesh C.; Silverton, J. V.
CS Frederick Cancer Res. Fac., Natl. Cancer Inst., Frederick, MD, 21701, USA
SO Journal of the American Chemical Society (1982), 104(16), 4478-9
CODEN: JACSAT; ISSN: 0002-7863

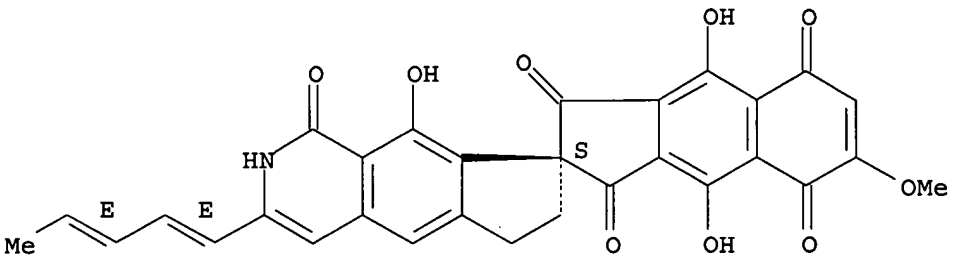
DT Journal
LA English
IT **80455-68-1**
RL: RCT (Reactant); RACT (Reactant or reagent)
(crystal structure and mol. structure of)
RN 80455-68-1 CAPLUS
CN Spiro[2H-benz[f]indene-2,8'-[8H]cyclopent[g]isoquinoline]-1,1',3,5,8(2'H)-pentone, 6',7'-dihydro-4,9,9'-trihydroxy-6-methoxy-3'-[(1E,3E)-1,3-pentadienyl]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



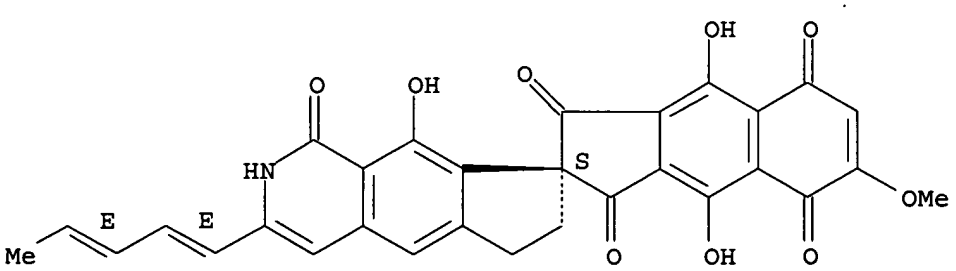
L8 ANSWER 120 OF 121 CAPLUS COPYRIGHT 2006 ACS on STN
AB A new antitumor antibiotic, fredericamycin A **[80455-68-1]**, was isolated from a strain of Streptomyces griseus (FCRC-48). Based on its unique UV-visible spectra, IR spectra, proton and 13C-NMR spectra and mass spectra, it is judged to be a novel acid-base indicator type of compound Its production, isolation, and physicochem. properties are discussed. The isolation, UV-visible spectra and some biol. properties of 2 minor components, fredericamycin B [80450-64-2] and fredericamycin C [80450-65-3], are also described.
AN 1982:84033 CAPLUS
DN 96:84033
TI Fredericamycin A, a new antitumor antibiotic. I. Production, isolation and physiocochemical properties
AU Pandey, Ramesh C.; Toussaint, Margaret W.; Stroshane, Ronald M.; Kalita, Chabi C.; Aszalos, Adorjan A.; Garretson, Aline L.; Wei, Tena T.; Byrne, Kevin M.; Geoghegan, Richard F., Jr.; White, Richard J.
CS Chemother. Ferment. Program, Frederick Cancer Res. Cent., Frederick, MD, 21701, USA
SO Journal of Antibiotics (1981), 34(11), 1389-401
CODEN: JANTAJ; ISSN: 0021-8820
DT Journal
LA English
IT **80455-68-1**
RL: BIOL (Biological study)
(antibiotic, from Streptomyces griseus)
RN 80455-68-1 CAPLUS
CN Spiro[2H-benz[f]indene-2,8'-[8H]cyclopent[g]isoquinoline]-1,1',3,5,8(2'H)-pentone, 6',7'-dihydro-4,9,9'-trihydroxy-6-methoxy-3'-[(1E,3E)-1,3-pentadienyl]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



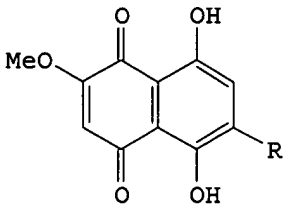
L8 ANSWER 121 OF 121 CAPLUS COPYRIGHT 2006 ACS on STN
AB fredericamycin A [**80455-68-1**], A novel antibiotic produced by a soil isolate of Streptomyces griseus (FCR-48), exhibits antibacterial, antifungal, and cytotoxic activities in vitro. In vivo, fredericamycin A exhibits very good antitumor activity against P388 mouse leukemia as well as the CD8F mammary tumor and marginal activity against B16 melanoma. Fredericamycin A failed to demonstrate any interaction with DNA, and inhibited protein and RNA synthesis preferentially to DNA synthesis in Bacillus subtilis and P388 cells.
AN 1982:62667 CAPLUS
DN 96:62667
TI Fredericamycin A, a new antitumor antibiotic. II. Biological properties
AU Warnick-Pickle, Dana J.; Byrne, Kevin M.; Pandey, Ramesh C.; White, Richard J.
CS Chemother. Ferment. Program, Frederick Cancer Res. Cent., Frederick, MD, 21701, USA
SO Journal of Antibiotics (1981), 34(11), 1402-7
CODEN: JANTAJ; ISSN: 0021-8820
DT Journal
LA English
IT **80455-68-1**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(as antibiotic, antibacterial and antifungal and antitumor activity of)
RN 80455-68-1 CAPLUS
CN Spiro[2H-benz[f]indene-2,8'-[8H]cyclopent[g]isoquinoline]-1,1',3,5,8(2'H)-pentone, 6',7'-dihydro-4,9,9'-trihydroxy-6-methoxy-3'-[(1E,3E)-1,3-pentadienyl]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

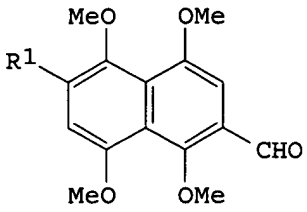


=> d abs bib hitstr 90-99

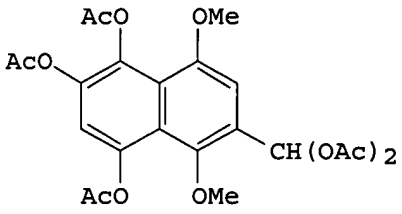
L8 ANSWER 90 OF 121 CAPLUS COPYRIGHT 2006 ACS on STN
GI



I



II

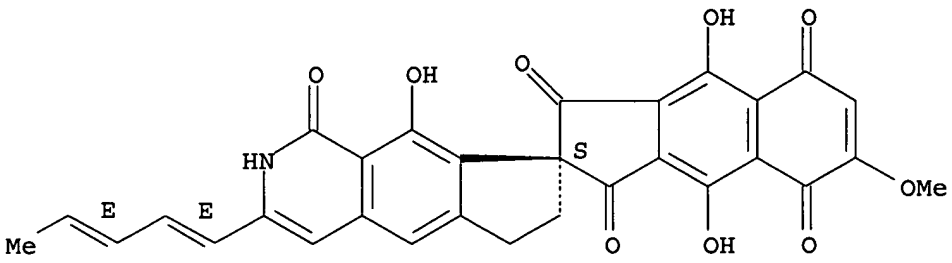


III

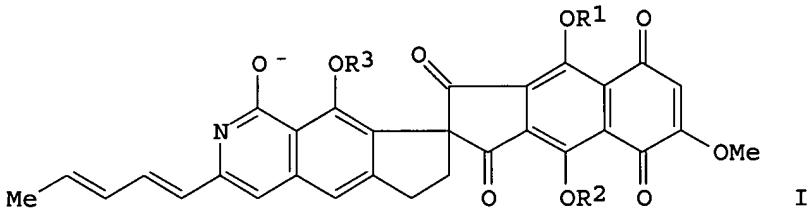
AB As potential intermediates for 2-methoxynaphthazarin antibiotics, naphthoquinones I(R = CHO, CH2OH) were prepared from tetramethoxynaphthalene II (R1 = H). Selective oxidative demethylation of II with ceric ammonium nitrate (CAN) gave an intermediate naphthoquinone which was treated with Ac2O-H2SO4 to give acetate III. Alkaline hydrolysis of III followed by methylation with Me2SO4 gave II (R1 = MeO) (IV). Oxidative demethylation of IV with CAN followed by further demethylation with AlCl3 gave I(R = CHO). I(R = CH2OH) was prepared from IV in 3 steps.

AN 1988:186289 CAPLUS
DN 108:186289
TI Synthesis of naphthoquinone derivatives. IV. Synthesis of 5,8-dihydroxy-2-methoxy-1,4-naphthoquinone derivatives. A major naphthoquinone moiety of some of naphthoquinone antibiotics
AU Tanoue, Yasuhiro; Terada, Akira; Tsuboi, Toshiyuki; Hayashida, Takayuki; Tsuge, Otohiko
CS Dep. Chem., Kyushu Inst. Technol., Kitakyushu, 804, Japan
SO Bulletin of the Chemical Society of Japan (1987), 60(8), 2927-30
CODEN: BCSJA8; ISSN: 0009-2673
DT Journal
LA English
OS CASREACT 108:186289
IT **80455-68-1**, Fredericamycin A
RL: RCT (Reactant); RACT (Reactant or reagent)
(dihydroxymethoxynaphthoquinone intermediate for, preparation of)
RN 80455-68-1 CAPLUS
CN Spiro[2H-benz[f]indene-2,8'-[8H]cyclopent[g]isoquinoline]-1,1',3,5,8(2'H)-pentone, 6',7'-dihydro-4,9,9'-trihydroxy-6-methoxy-3'-[(1E,3E)-1,3-pentadienyl]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



L8 ANSWER 91 OF 121 CAPLUS COPYRIGHT 2006 ACS on STN
GI



I

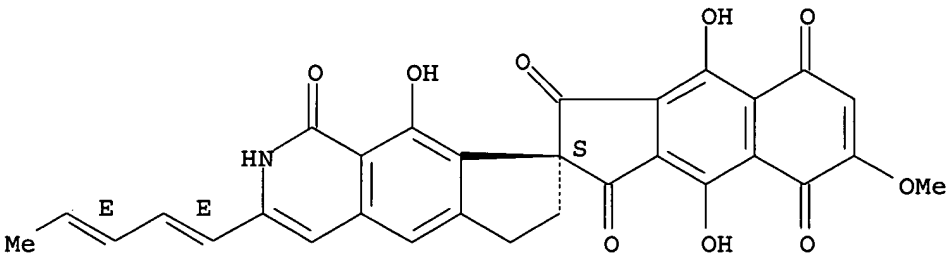
AB The title compds. I (1 of R1, R2, R3 = alkali metal and the others = H, alkali metal) were prepared as antimicrobial and antitumor agents by neutralization of 1 or more phenolic groups with alkali metal hydroxides. Thus, 0.2781 mmol KOH was added at 0° to 0.0959 mmol fredericamycin A in pyridine degassed with N and stirred 1 h whereupon the solution is lyophilized. The compound (II) thus obtained is stable for several months at 1° in a dry atmospheric At 1 mg/kg i.p. II increased survival of mice inoculated with P388 leukemia cells 78% over controls.
AN 1988:167205 CAPLUS
DN 108:167205
TI Preparation of water soluble derivatives of fredericamycin A as antimicrobial and antitumor agents
IN Misra, R.
PA United States Dept. of Health and Human Services, USA
SO U. S. Pat. Appl., 28 pp. Avail. NTIS Order No. PAT-APPL-6-889 501.
CODEN: XAXXAV
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 889501	A0	19861205	US 1986-889501	19860725
US 4673678	A	19870616		
PRAI US 1986-889501		19860725		

OS MARPAT 108:167205
IT **80455-68-1P**, Fredericamycin A **113974-30-4P**
113974-31-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as antimicrobial and antitumor agent)
RN 80455-68-1 CAPLUS
CN Spiro[2H-benz[f]indene-2,8'-[8H]cyclopent[g]isoquinoline]-1,1',3,5,8(2'H)-pentone, 6',7'-dihydro-4,9,9'-trihydroxy-6-methoxy-3'-[(1E,3E)-1,3-

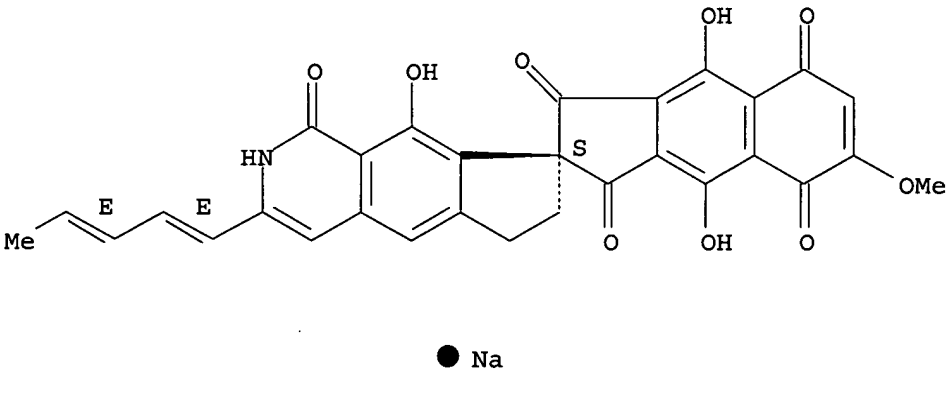
pentadienyl]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



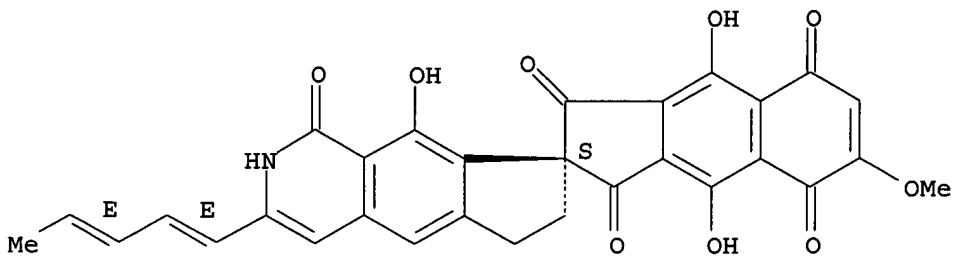
RN 113974-30-4 CAPLUS
CN Spiro[2H-benz[f]indene-2,8'-[8H]cyclopent[g]isoquinoline]-1,1',3,5,8(2'H)-pentone, 6',7'-dihydro-4,9,9'-trihydroxy-6-methoxy-3'-[(1E,3E)-1,3-pentadienyl]-, monosodium salt, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



RN 113974-31-5 CAPLUS
CN Spiro[2H-benz[f]indene-2,8'-[8H]cyclopent[g]isoquinoline]-1,1',3,5,8(2'H)-pentone, 6',7'-dihydro-4,9,9'-trihydroxy-6-methoxy-3'-[(1E,3E)-1,3-pentadienyl]-, monopotassium salt, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



● K

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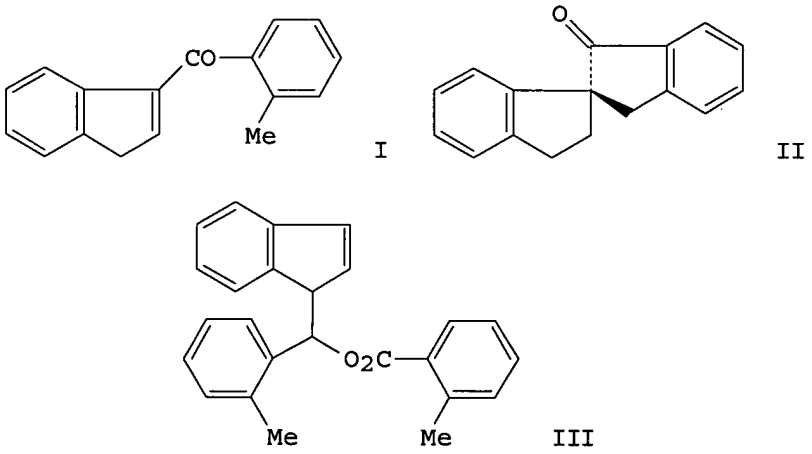


AB Novel photochem. of $\pi\pi^*$ triplet of enone I has been applied to the synthesis of a model spiro compound II related to fredericamycin A. Phase-transfer catalyst, e.g. Bu4NBr was used for the ditoluylation of indene, leading to enol ester III which was hydrolyzed to I.

AN 1988:75065 CAPLUS

DN 108:75065

TI A novel photochemical strategy for a model spiro compound related to fredericamycin A

AU Khire, U. R.; Naik, S. N.; Pandey, B.; Ayyangar, N. R.

CS Natl. Chem. Lab., Pune, 411 008, India

SO Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1987), 26B(3), 195-6
CODEN: IJSBDB; ISSN: 0376-4699

DT Journal

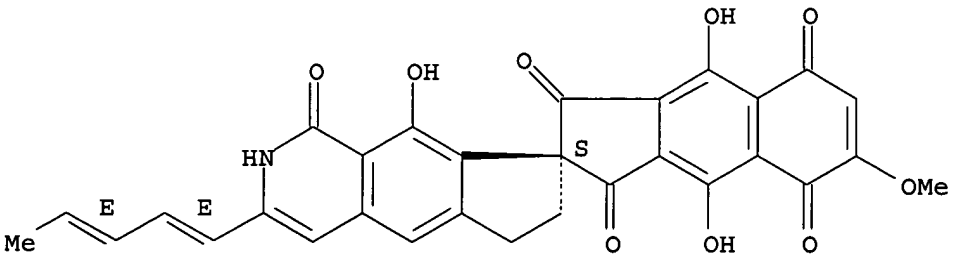
LA English

OS CASREACT 108:75065

IT **80455-68-1**, Fredericamycin A
RL: RCT (Reactant); RACT (Reactant or reagent)

(model compound for, photochem. preparation of)
RN 80455-68-1 CAPLUS
CN Spiro[2H-benz[f]indene-2,8'-[8H]cyclopent[g]isoquinoline]-1,1',3,5,8(2'H)-pentone, 6',7'-dihydro-4,9,9'-trihydroxy-6-methoxy-3'-[(1E,3E)-1,3-pentadienyl]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



L8 ANSWER 93 OF 121 CAPLUS COPYRIGHT 2006 ACS on STN
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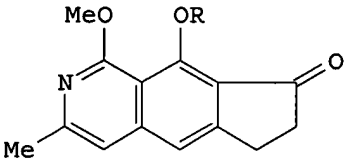

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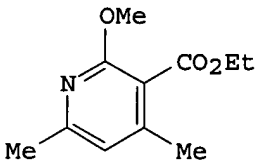
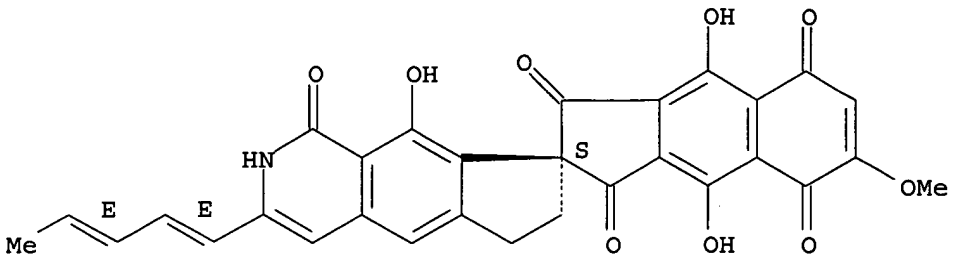


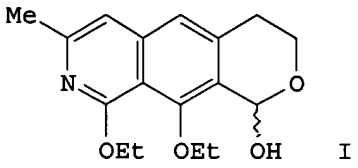
II

AB Cyclopent[g]isoquinoline fragments I (R = H, Me) of fredericamycin A were prepared by directed lithiation of pyridine II and conjugate addition to 2-cyclopenten-1-one. Cyclization of the product with base then generated the required skeleton, which was aromatized and methylated to I.
AN 1988:55719 CAPLUS
DN 108:55719
TI Synthesis of heterocyclic compounds related to fredericamycin A. The cyclopent[g]isoquinoline system
AU Clive, Derrick L. J.; Sedgeworth, Janette
CS Chem. Dep., Univ. Alberta, Edmonton, AB, T6G 2G2, Can.
SO Journal of Heterocyclic Chemistry (1987), 24(2), 509-11
CODEN: JHTCAD; ISSN: 0022-152X
DT Journal
LA English
OS CASREACT 108:55719
IT **80455-68-1P**, Fredericamycin A
RL: SPN (Synthetic preparation); PREP (Preparation)
(cyclopentisoquinoline fragment of, preparation of)
RN 80455-68-1 CAPLUS
CN Spiro[2H-benz[f]indene-2,8'-[8H]cyclopent[g]isoquinoline]-1,1',3,5,8(2'H)-pentone, 6',7'-dihydro-4,9,9'-trihydroxy-6-methoxy-3'-[(1E,3E)-1,3-pentadienyl]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



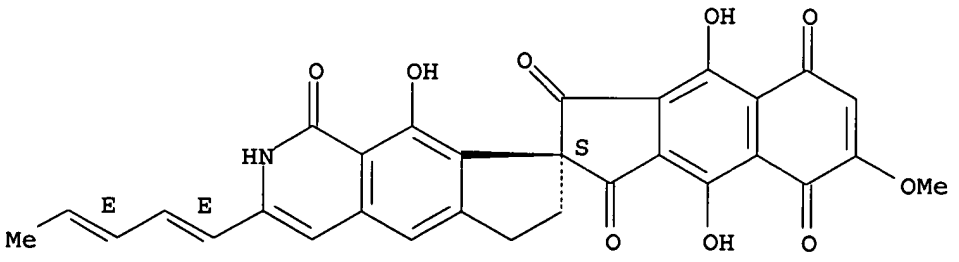
L8 ANSWER 94 OF 121 CAPLUS COPYRIGHT 2006 ACS on STN
GI



I

AB The isoquinoline I, comprising of the DEF rings in fredericamycin A, has been prepared in 7 steps starting from 4-methyl-5-ethoxyoxazole.
AN 1987:636309 CAPLUS
DN 107:236309
TI Synthesis of 3-methyl-6-(2-hydroxyethyl)-7-formyl-1,8-diethoxyisoquinoline. A key synthon for fredericamycin A
AU Rao, A. V. Rama; Reddy, D. Reddeppa
CS Reg. Res. Lab., Hyderabad, 500 007, India
SO Journal of the Chemical Society, Chemical Communications (1987), (8), 574-5
CODEN: JCCCAT; ISSN: 0022-4936
DT Journal
LA English
OS CASREACT 107:236309
IT **80455-68-1P**, Fredericamycin A
RL: SPN (Synthetic preparation); PREP (Preparation)
(isoquinoline fragment of, preparation of)
RN 80455-68-1 CAPLUS
CN Spiro[2H-benz[f]indene-2,8'-[8H]cyclopent[g]isoquinoline]-1,1',3,5,8(2'H)-pentone, 6',7'-dihydro-4,9,9'-trihydroxy-6-methoxy-3'-[(1E,3E)-1,3-pentadienyl]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



L8 ANSWER 95 OF 121 CAPLUS COPYRIGHT 2006 ACS on STN
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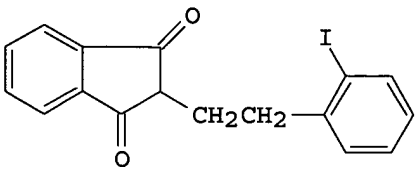

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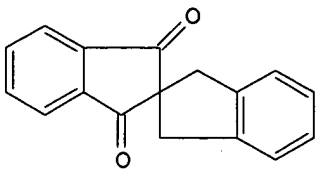
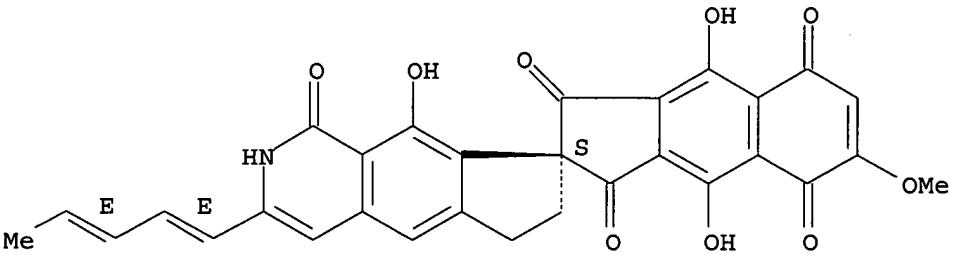


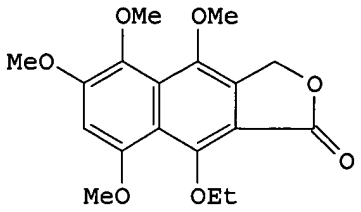
II

AB The Pd(PPh3)4-promoted intramol. arylation of the β-diketone I generates the spirocyclic system II as a model for fredericamycin A.
AN 1987:636294 CAPLUS
DN 107:236294
TI Efficient palladium-mediated synthesis of a spirocyclic model for fredericamycin A
AU Ciufolini, Marco A.; Browne, Margaret E.
CS Dep. Chem., Rice Univ., Houston, TX, 77251, USA
SO Tetrahedron Letters (1987), 28(2), 171-4
CODEN: TELEAY; ISSN: 0040-4039
DT Journal
LA English
OS CASREACT 107:236294
IT **80455-68-1**, Fredericamycin A
RL: RCT (Reactant); RACT (Reactant or reagent)
(spirobiindandione model for, preparation of)
RN 80455-68-1 CAPLUS
CN Spiro[2H-benz[f]indene-2,8'-[8H]cyclopent[g]isoquinoline]-1,1',3,5,8(2'H)-pentone, 6',7'-dihydro-4,9,9'-trihydroxy-6-methoxy-3'-[(1E,3E)-1,3-pentadienyl]-, (2S)- (9CI) (CA INDEX NAME)

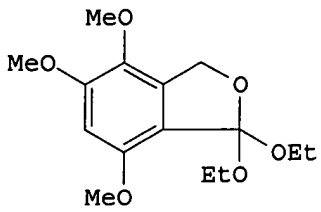
Absolute stereochemistry.
Double bond geometry as shown.



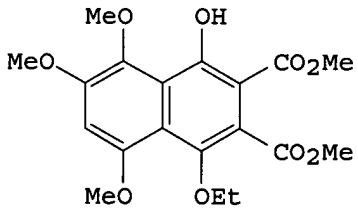
L8 ANSWER 96 OF 121 CAPLUS COPYRIGHT 2006 ACS on STN
GI



I



III



IV

AB Lactone I, as a synthon for the ABC rings of fredericamycin A, was prepared regiospecifically from 3,5-(HO)2C6H3CO2H (II). Orthoester III, prepared in several steps from II, was treated with AcOH to generate a diene in situ which underwent cycloaddn. with MeO2CC.tplbond.CCO2Me to give naphthol IV. Further elaboration of IV gave I.

AN 1987:534091 CAPLUS

DN 107:134091

TI Regiospecific synthesis of 9-ethoxy-4,5,6,8-tetramethoxy-1,3-dihydronaphtho(2,3-c)furan-1-one: a key synthon of fredericamycin A

AU Rao, A. V. Rama; Sreenivasan, N.; Reddy, D. Reddeppa; Deshpande, V. H.

CS Natl. Chem. Lab., Pune, 411 008, India

SO Tetrahedron Letters (1987), 28(4), 455-8
CODEN: TELEAY; ISSN: 0040-4039

DT Journal

LA English

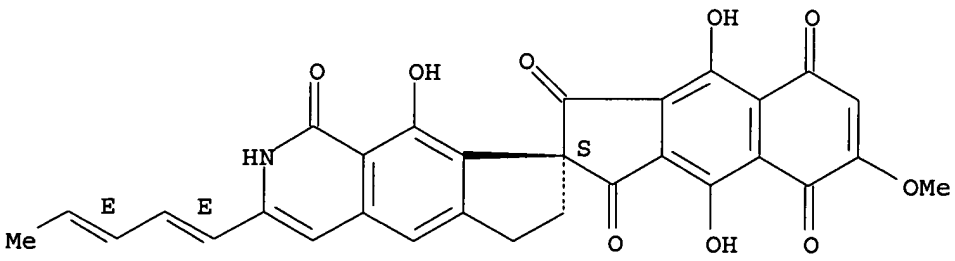
OS CASREACT 107:134091

IT **80455-68-1P**, Fredericamycin A
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of ring synthon of)

RN 80455-68-1 CAPLUS

CN Spiro[2H-benz[f]indene-2,8'-[8H]cyclopent[g]isoquinoline]-1,1',3,5,8(2'H)-pentone, 6',7'-dihydro-4,9,9'-trihydroxy-6-methoxy-3'-[(1E,3E)-1,3-pentadienyl]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



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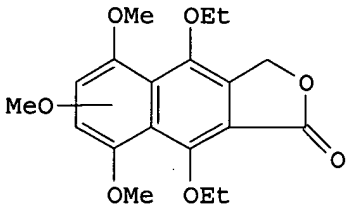

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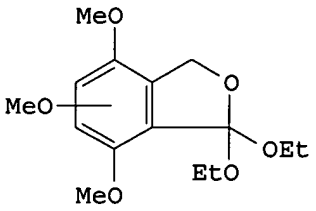
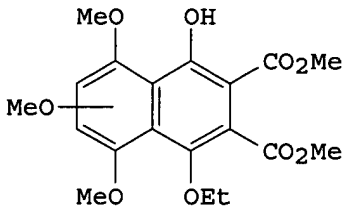


III



IV

AB The title furanone I, a synthon for the ABC rings of fredericamycin A, was prepared from vanillin (II). In a key reaction, ortho ester III, prepared in several steps from II, was treated with AcOH to generate a diene in situ, which underwent cycloaddn. with MeO2CC.tplbond.CCO2Me to give naphthalenedicarboxylate IV. Further elaboration of IV gave I.

AN 1987:534090 CAPLUS

DN 107:134090

TI Synthesis of 4,9-diethoxy-5,6(7),8-trimethoxy-1,3-dihydronaphtho(2,3-c)furan-1-one: a key synthon of fredericamycin A

AU Rao, A. V. Rama; Reddy, D. Reddeppa; Annapurna, G. S.; Deshpande, V. H.

CS Natl. Chem. Lab., Pune, 411 008, India

SO Tetrahedron Letters (1987), 28(4), 451-4
CODEN: TELEAY; ISSN: 0040-4039

DT Journal

LA English

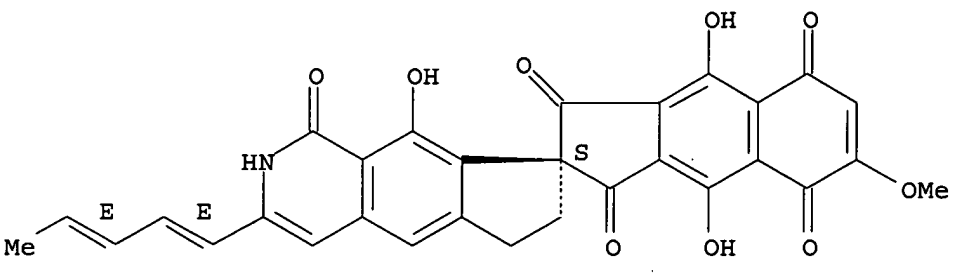
OS CASREACT 107:134090

IT **80455-68-1P**, Fredericamycin A
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of ring synthon of)

RN 80455-68-1 CAPLUS

CN Spiro[2H-benz[f]indene-2,8'-[8H]cyclopent[g]isoquinoline]-1,1',3,5,8(2'H)-pentone, 6',7'-dihydro-4,9,9'-trihydroxy-6-methoxy-3'-[(1E,3E)-1,3-pentadienyl]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



L8 ANSWER 98 OF 121 CAPLUS COPYRIGHT 2006 ACS on STN
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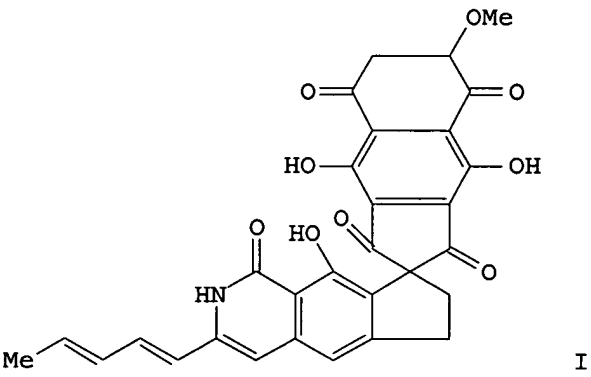


I

AB IR, UV-visible spectroscopy, CD, 1H and 13C NMR studies, high resolution electron impact, field desorption, and fast atom bombardment mass spectral studies are reported for fredericamycin A (NSC-305263) (I), a novel antitumor antibiotic of acid-base indicator type produced by Streptomyces griseus (FCRC-48). The spectral data are correlated with the structure obtained by X-ray crystallog. The novel spiro ring antibiotic exhibits unusual 1H and 13C NMR spectroscopic and chemical behavior, not previously observed in other antibiotic structures.

AN 1987:515412 CAPLUS

DN 107:115412

TI Structure of fredericamycin A, an antitumor antibiotic of a novel skeletal type; spectroscopic and mass spectral characterization

AU Misra, Renuka; Pandey, Ramesh C.; Hilton, Bruce D.; Roller, Peter P.; Silverton, James V.

CS Frederick Cancer Res. Facil., Natl. Cancer Inst., Frederick, MD, 21701, USA

SO Journal of Antibiotics (1987), 40(6), 786-802
CODEN: JANTAJ; ISSN: 0021-8820

DT Journal

LA English

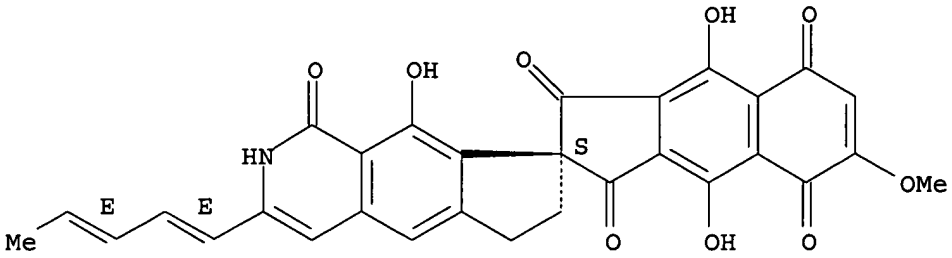
IT **80455-68-1**, Fredericamycin A
RL: PRP (Properties)
(structure of)

RN 80455-68-1 CAPLUS

CN Spiro[2H-benz[f]indene-2,8'-[8H]cyclopent[g]isoquinoline]-1,1',3,5,8(2'H)-

pentone, 6',7'-dihydro-4,9,9'-trihydroxy-6-methoxy-3'-[(1E,3E)-1,3-pentadienyl]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



L8 ANSWER 99 OF 121 CAPLUS COPYRIGHT 2006 ACS on STN
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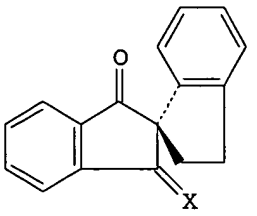
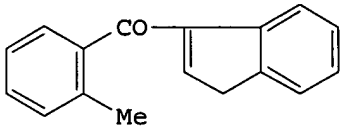
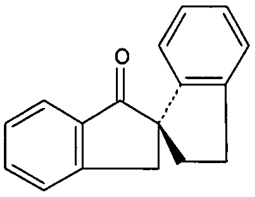


I



II



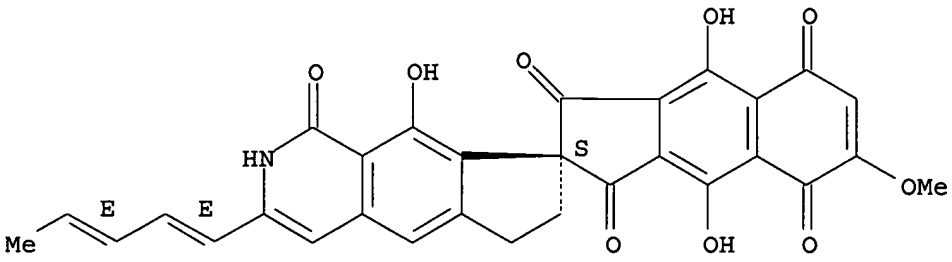
III

AB As a model for fredericamycin A synthesis, spirodione I (X = O) was prepared by a photochem. cyclization of indene II to give spiroketone III. Conversion of III to benzylidene derivative I (X = PhCH) followed by oxidative cleavage gave I (X = O). Condensation of indene with o-MeC6H4COCl followed by isomerization gave II.

AN 1987:477492 CAPLUS
DN 107:77492
TI Model studies towards fredericamycin A. Protocol for the rapid creation of the spirocyclic center
AU Mehta, Goverdhan; Subrahmanyam, Duvvuri
CS Sch. Chem., Univ. Hyderabad, Hyderabad, 500 134, India
SO Tetrahedron Letters (1987), 28(4), 479-80
CODEN: TELEAY; ISSN: 0040-4039
DT Journal
LA English
OS CASREACT 107:77492
IT **80455-68-1P**, Fredericamycin A

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of spirocyclic center of)
RN 80455-68-1 CAPLUS
CN Spiro[2H-benz[f]indene-2,8'-[8H]cyclopent[g]isoquinoline]-1,1',3,5,8(2'H)-pentone, 6',7'-dihydro-4,9,9'-trihydroxy-6-methoxy-3'-[(1E,3E)-1,3-pentadienyl]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



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FULL ESTIMATED COST	0.12	504.17

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